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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS 3	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS 4	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS 5	APR 28	IMSRESEARCH reloaded with enhancements
NEWS 6	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS 7	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS 8	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS 9	JUN 06	KOREAPAT updated with 41,000 documents
NEWS 10	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS 11	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS 12	JUN 25	CA/CAplus and USPAT databases updated with IPC reclassification data
NEWS 13	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS 14	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS 15	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS 16	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS 17	JUL 28	CA/CAplus patent coverage enhanced
NEWS 18	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS 19	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 20	JUL 28	STN Viewer performance improved
NEWS 21	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS 22	AUG 13	CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS 23	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 24	AUG 15	CAplus currency for Korean patents enhanced
NEWS 25	AUG 25	CA/CAplus, CASREACT, and IFI and USPAT databases enhanced for more flexible patent number searching
NEWS 26	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,

AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:26:32 ON 10 SEP 2008

=> FIL REG
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 12:26:47 ON 10 SEP 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 SEP 2008 HIGHEST RN 1048111-29-0
DICTIONARY FILE UPDATES: 9 SEP 2008 HIGHEST RN 1048111-29-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

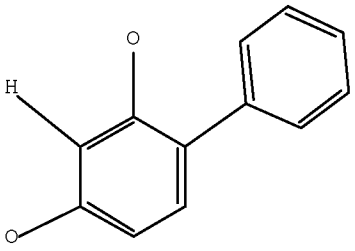
http://www.cas.org/support/stngen/stndoc/properties.html

=> ACTIVATE KITA10584234/A
L1 STR
L2 825 SEA FILE=REGISTRY SSS FUL L1

=> ACTIVATE KI10584234/A
L3 STR
L4 (3163) SEA FILE=REGISTRY SSS FUL L3
L5 STR
L6 1721 SEA FILE=REGISTRY SUB=L4 SSS FUL L5

=> D L3

L3 HAS NO ANSWERS
L3 STR



Structure attributes must be viewed using STN Express query preparation.

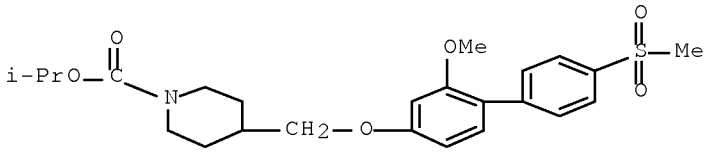
=> D L5
L5 HAS NO ANSWERS
L5 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> D SCAN L6

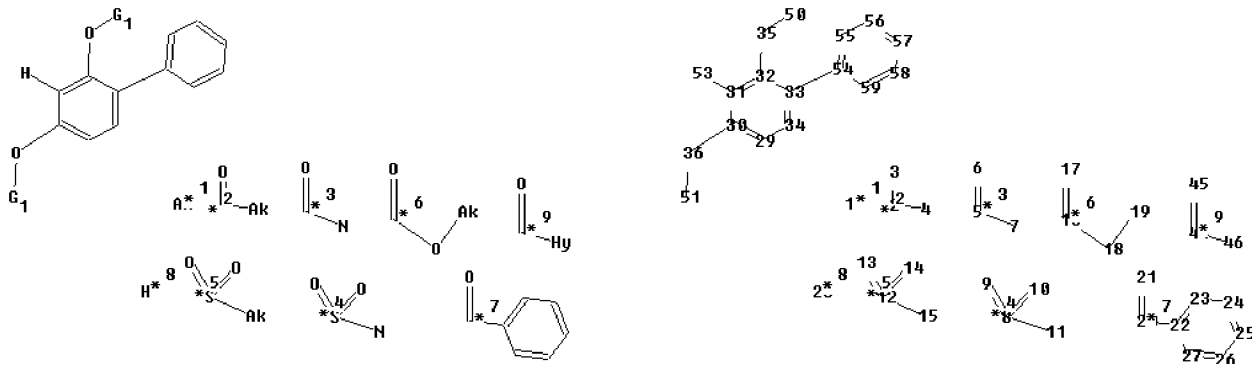
L6 1721 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1-Piperidinecarboxylic acid, 4-[[[2-methoxy-4'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]oxy]methyl]-, 1-methylethyl ester
MF C24 H31 N O6 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>
Uploading C:\Program Files\STNEXP\Queries\10584234NN.str



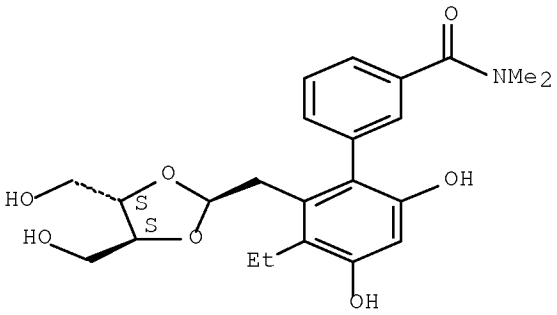
chain nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 28 35
36 44 45 46 50 51 53
ring nodes :
22 23 24 25 26 27 29 30 31 32 33 34 54 55 56 57 58 59
chain bonds :
2-3 2-4 5-6 5-7 8-9 8-10 8-11 12-13 12-14 12-15 16-17 16-18 18-19 20-21
20-22 30-36 31-53 32-35 33-54 35-50 36-51 44-45 44-46
ring bonds :
22-23 22-27 23-24 24-25 25-26 26-27 29-30 29-34 30-31 31-32 32-33 33-34
54-55 54-59 55-56 56-57 57-58 58-59
exact/norm bonds :
2-3 2-4 5-6 5-7 8-9 8-10 8-11 12-13 12-14 12-15 16-17 16-18 18-19 20-21
30-36 32-35 35-50 36-51 44-45 44-46
exact bonds :
20-22 31-53 33-54
normalized bonds :
22-23 22-27 23-24 24-25 25-26 26-27 29-30 29-34 30-31 31-32 32-33 33-34
54-55 54-59 55-56 56-57 57-58 58-59

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS
29:Atom 30:Atom
31:Atom 32:Atom 33:Atom 34:Atom 35:CLASS 36:CLASS 44:CLASS 45:CLASS 46:Atom
50:CLASS
51:CLASS 53:CLASS 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom
Generic attributes :
1:
Saturation : Unsaturated

L7 STRUCTURE UPLOADED

```
=> D L7
L7 HAS NO ANSWERS
L7              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> S SSS SAM L7
SAMPLE SEARCH INITIATED 12:31:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     5070 TO ITERATE

 39.4% PROCESSED     2000 ITERATIONS                              25 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         97130 TO   105670
PROJECTED ANSWERS:              790 TO     1744

L8           25 SEA SSS SAM L7

=> D SCAN

L8   25 ANSWERS   REGISTRY  COPYRIGHT 2008 ACS on STN
IN   6,8-Isoquinolinediol, 1,2,3,4-tetrahydro-5-(4-hydroxy-5-methoxy-7-methyl-1-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S SSS SAM L7 SUBSET=L6
SAMPLE SUBSET SEARCH INITIATED 12:32:13 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -       92 TO ITERATE

100.0% PROCESSED       92 ITERATIONS                              18 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):           ONLINE  **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):         1265 TO     2415
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):             106 TO      614

L9           18 SEA SUB=L6 SSS SAM L7

=> D SCAN

L9   18 ANSWERS   REGISTRY  COPYRIGHT 2008 ACS on STN
IN   [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3-
     dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N,N-dimethyl-
MF   C23 H29 N O7

Absolute stereochemistry.
```



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S SSS FULL L7 SUBSET=L6
FULL SUBSET SEARCH INITIATED 12:32:33 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1721 TO ITERATE

100.0% PROCESSED 1721 ITERATIONS 368 ANSWERS
SEARCH TIME: 00.00.01

L10 368 SEA SUB=L6 SSS FUL L7

=> FIL CAPLU

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	46.70	46.91

FILE 'CAPLUS' ENTERED AT 12:32:48 ON 10 SEP 2008

FILE COVERS 1907 - 10 Sep 2008 VOL 149 ISS 11
FILE LAST UPDATED: 9 Sep 2008 (20080909/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

```
=> S L10
L11        160 L10

=> S L11 AND (AY<20O3 OR PY<2003 OR PRY<2003)
NUMERIC VALUE NOT VALID '20O3'
Numeric values may contain 1-8 significant figures.  If range notation
is used, both the beginning and the end of the range must be
specified, e.g., '250-300/MW'.  Expressions such as '250-/MW' are not
allowed.  To search for values above or below a given number, use the
>, =>, <, or <= operators, e.g., 'MW => 250'.  Text terms cannot be
used in numeric expressions.  If you specify a unit, it must be
dimensionally correct for that field code.  To see the unit
designations for field codes in the current file, enter "DISPLAY UNIT
ALL" at an arrow prompt (=>).

=> S L11 AND (AY<20O3 OR PY<2003 OR PRY<2003)
NUMERIC VALUE NOT VALID '20O3'
Numeric values may contain 1-8 significant figures.  If range notation
is used, both the beginning and the end of the range must be
specified, e.g., '250-300/MW'.  Expressions such as '250-/MW' are not
allowed.  To search for values above or below a given number, use the
>, =>, <, or <= operators, e.g., 'MW => 250'.  Text terms cannot be
used in numeric expressions.  If you specify a unit, it must be
dimensionally correct for that field code.  To see the unit
designations for field codes in the current file, enter "DISPLAY UNIT
ALL" at an arrow prompt (=>).

=> S l11 and (ay<2003 or py<2003 or pry<2003)
       4496803 AY<2003
      22958877 PY<2003
       3965143 PRY<2003
L12        135 L11 AND (AY<2003 OR PY<2003 OR PRY<2003)

=> S l11 and (ay<2004 or py<2004 or pry<2004)
       4785567 AY<2004
      24009596 PY<2004
       4256742 PRY<2004
L13        145 L11 AND (AY<2004 OR PY<2004 OR PRY<2004)

=> l13 and HSP
L13 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s l13 and HSP
         23728 HSP
          2831 HSPS
         24314 HSP
                 (HSP OR HSPS)
L14          2 L13 AND HSP

=> fil stng
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               26.36      73.27

FILE 'STNGUIDE' ENTERED AT 12:47:26 ON 10 SEP 2008
```

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Sep 5, 2008 (20080905/UP).

=> FIL REGISTRY
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   0.06   73.33

FILE 'REGISTRY' ENTERED AT 12:47:58 ON 10 SEP 2008

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 9 SEP 2008 HIGHEST RN 1048111-29-0
DICTIONARY FILE UPDATES: 9 SEP 2008 HIGHEST RN 1048111-29-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d his

     (FILE 'HOME' ENTERED AT 12:26:32 ON 10 SEP 2008)

     FILE 'REGISTRY' ENTERED AT 12:26:47 ON 10 SEP 2008
                ACTIVATE KITA10584234/A

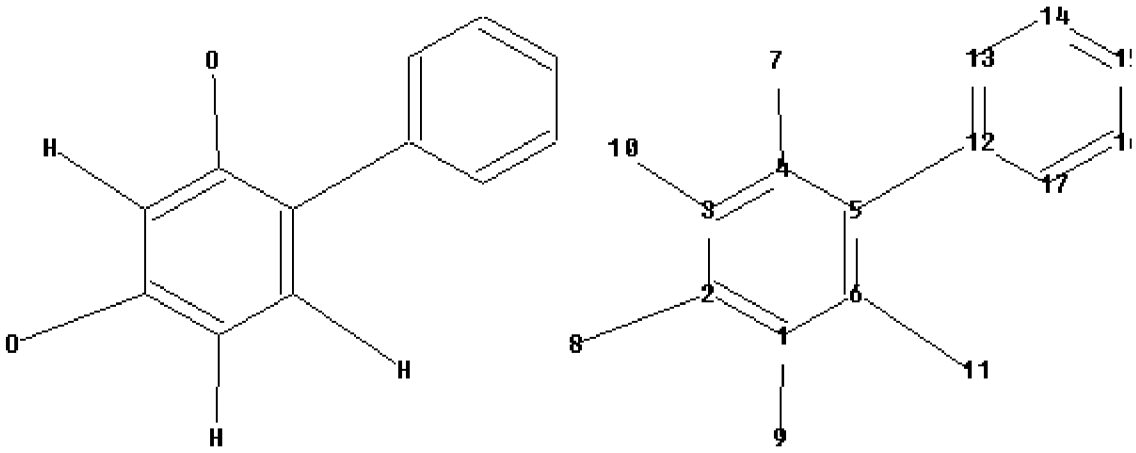
L1   STR
L2   825 SEA FILE=REGISTRY SSS FUL L1

                ACTIVATE KI10584234/A

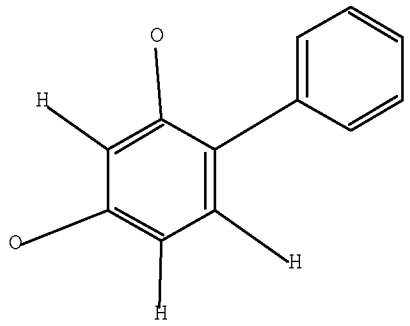
L3   STR
L4   (3163)SEA FILE=REGISTRY SSS FUL L3
L5   STR
L6   1721 SEA FILE=REGISTRY SUB=L4 SSS FUL L5

L7   STRUCTURE UPLOADED
L8   25 S SSS SAM L7
L9   18 S SSS SAM L7 SUB=L6
L10   368 S SSS FULL L7 SUB=L6

```
     FILE 'CAPLUS' ENTERED AT 12:32:48 ON 10 SEP 2008
L11          160 S L10
L12          135 S L11 AND (AY<2003 OR PY<2003 OR PRY<2003)
L13          145 S L11 AND (AY<2004 OR PY<2004 OR PRY<2004)
L14            2 S L13 AND HSP

     FILE 'STNGUIDE' ENTERED AT 12:47:26 ON 10 SEP 2008

     FILE 'REGISTRY' ENTERED AT 12:47:58 ON 10 SEP 2008

=>
Uploading C:\Program Files\STNEXP\Queries\10584234OO.str
```




```
chain nodes :
7  8  9  10  11
ring nodes :
1  2  3  4  5  6  12  13  14  15  16  17
chain bonds :
1-9  2-8  3-10  4-7  5-12  6-11
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  12-13  12-17  13-14  14-15  15-16  16-17
exact/norm bonds :
2-8  4-7
exact bonds :
1-9  3-10  5-12  6-11
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  12-13  12-17  13-14  14-15  15-16  16-17


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom



L15     STRUCTURE UPLOADED

=> d l15
L15 HAS NO ANSWERS
L15             STR
```



Structure attributes must be viewed using STN Express query preparation.

```
=> s sss sam l15 subset=l10
SAMPLE SUBSET SEARCH INITIATED 12:54:05 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -       18 TO ITERATE

100.0% PROCESSED       18 ITERATIONS                              8 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):           ONLINE  **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):          106 TO      614
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):               8 TO      329

L16           8 SEA SUB=L10 SSS SAM L15

=> d scan

ALL ANSWERS HAVE BEEN SCANNED


=> s sss full l15 subset=l10
FULL SUBSET SEARCH INITIATED 12:54:30 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -      368 TO ITERATE

100.0% PROCESSED      368 ITERATIONS                            145 ANSWERS
SEARCH TIME: 00.00.01

L17         145 SEA SUB=L10 SSS FUL L15

=> s l10 not l17
L18        223 L10 NOT L17

=> d scan


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      49.62     122.95
```

FILE 'CAPLUS' ENTERED AT 12:55:20 ON 10 SEP 2008
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FILE COVERS 1907 - 10 Sep 2008 VOL 149 ISS 11
FILE LAST UPDATED: 9 Sep 2008 (20080909/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

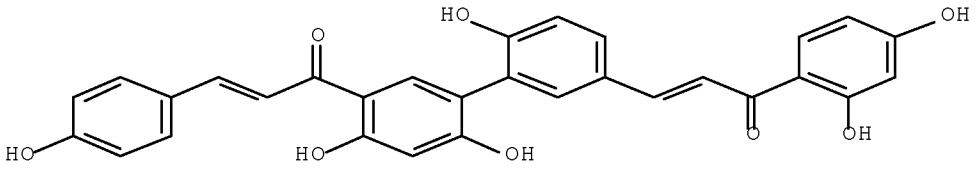
```
=> s l18
L19         52 L18

=> S l19 and (ay<2004 or py<2004 or pry<2004)
       4785567 AY<2004
      24009596 PY<2004
       4256742 PRY<2004
L20         47 L19 AND (AY<2004 OR PY<2004 OR PRY<2004)

=> d ibib abs hitstr l19

L19  ANSWER 1 OF 52  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        2008:122442  CAPLUS  Full-text
DOCUMENT NUMBER:         148:421710
TITLE:                   Secondary metabolites from Caesalpinia pluviosa
AUTHOR(S):               Flores, Yonny; Vila, Jose; Almanza, Giovanna R.
CORPORATE SOURCE:        Laboratorio de Productos Naturales, Instituto de
                         Investigaciones Quimicas, Carrera de Ciencias
                         Quimicas, Universidad Mayor de San Andres, La Paz,
                         Bolivia
SOURCE:                  Revista Boliviana de Quimica (2006), 23(1), 1-8
                         CODEN: RBQUDX; ISSN: 0250-5460
PUBLISHER:               Universidad Mayor de San Andres, Facultad de Ciencias
                         Puras y Naturales
DOCUMENT TYPE:           Journal
LANGUAGE:                English
AB    Two phenolic compds., Et gallate and rhuschalcone VI, together with lupeol,
      betulinic acid and stigmasterol were isolated from the stem bark of
      Caesalpinia pluviosa D.C.  Their structures were determined by spectroscopic
      means mainly by NMR expts., completing all the NMR assignments of phenolic
      compds.  In addition, the exts. and pure compds. were evaluated against the
      bacteria Staphylococcus aureus, HPIA test and the antimalarial in vitro assay
```

against Plasmodium falciparum, determining that CH2Cl2 extract and rhuschalcone VI showed good activity in the antibacterial and HPIA tests.

IT 541502-84-5P, Rhuschalcone VI
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(secondary metabolites from Caesalpinia pluviosa)

RN 541502-84-5 CAPLUS

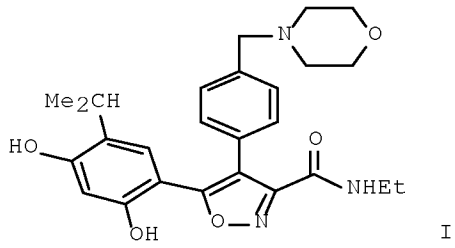
CN 2-Propen-1-one, 1-[5'-[(1E)-3-(2,4-dihydroxyphenyl)-3-oxo-1-propen-1-yl]-2',4,6-trihydroxy[1,1'-biphenyl]-3-yl]-3-(4-hydroxyphenyl)-, (2E)-(-)- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr l19 2-52

L19 ANSWER 2 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1319216 CAPLUS Full-text
DOCUMENT NUMBER: 148:144683
TITLE: 4,5-Diarylisoxazole Hsp90 Chaperone Inhibitors: Potential Therapeutic Agents for the Treatment of Cancer
AUTHOR(S): Brough, Paul A.; Aherne, Wynne; Barril, Xavier; Borgognoni, Jennifer; Boxall, Kathy; Cansfield, Julie E.; Cheung, Kwai-Ming J.; Collins, Ian; Davies, Nicholas G. M.; Drysdale, Martin J.; Dymock, Brian; Eccles, Suzanne A.; Finch, Harry; Fink, Alexandra; Hayes, Angela; Howes, Robert; Hubbard, Roderick E.; James, Karen; Jordan, Allan M.; Lockie, Andrea; Martins, Vanessa; Massey, Andrew; Matthews, Thomas P.; McDonald, Edward; Northfield, Christopher J.; Pearl, Laurence H.; Prodromou, Chrisostomos; Ray, Stuart; Raynaud, Florence I.; Roughley, Stephen D.; Sharp, Swee Y.; Surgenor, Allan; Walmsley, D. Lee; Webb, Paul; Wood, Mike; Workman, Paul; Wright, Lisa
CORPORATE SOURCE: Vernalis Ltd., Cambridge, CB21 6GB, UK
SOURCE: Journal of Medicinal Chemistry (2008), 51(2), 196-218
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



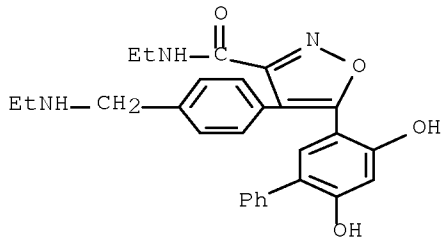
I

AB Inhibitors of the Hsp90 [heat shock protein 90] mol. chaperone show considerable promise as potential chemotherapeutic agents for cancer. The structure-based design, synthesis, structure-activity relationships, and pharmacokinetics of potent small-mol. inhibitors of Hsp90 based on the 4,5-diarylisoxazole scaffold were studied. Analogs from this series have high affinity for Hsp90, as measured in a fluorescence polarization competitive binding assay, and are active in cancer cell lines where they inhibit proliferation and exhibit a characteristic profile of depletion of oncogenic proteins and concomitant elevation of Hsp72. The [(morpholinomethyl)phenyl]isoxazolecarboxamide I (VER-52296/NVP-AUY922) is potent in the Hsp90 FP binding assay and inhibits proliferation of various human cancer cell lines in vitro, with GI50 averaging 9 nM. I is retained in tumors in vivo when administered i.p., as evaluated by cassette dosing in tumor-bearing mice. In a human colon cancer xenograft model, I inhibits tumor growth by .apprx.50%.

IT 1001386-05-5
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of diphenylisoxazolecarboxamides and diphenylpyrazolecarboxamides as heat shock protein chaperone inhibitors and anticancer agents)

RN 1001386-05-5 CAPLUS

CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-[(ethylamino)methyl]phenyl]- (CA INDEX NAME)

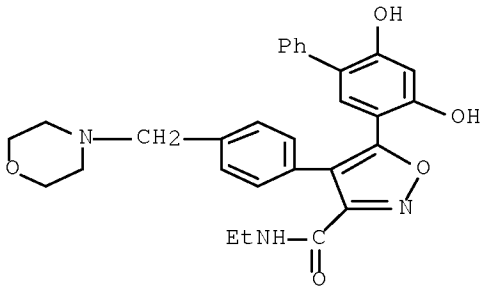


IT 747412-71-1P 747413-82-7P 747413-88-3P
747413-92-9P 747413-98-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of diphenylisoxazolecarboxamides and diphenylpyrazolecarboxamides as heat shock protein chaperone inhibitors and anticancer agents)

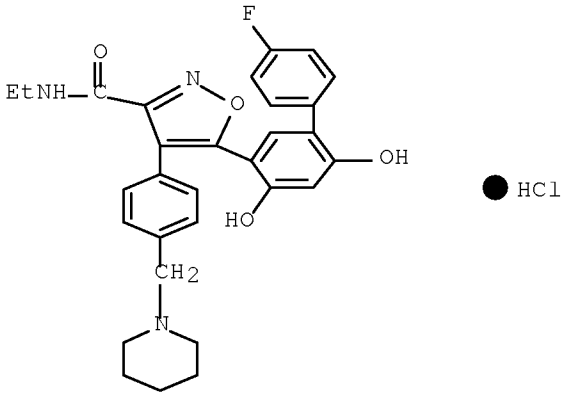
RN 747412-71-1 CAPLUS

CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-

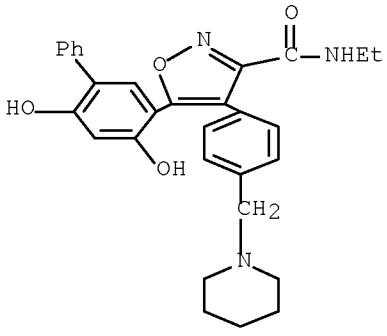
(4-morpholinylmethyl)phenyl]- (CA INDEX NAME)



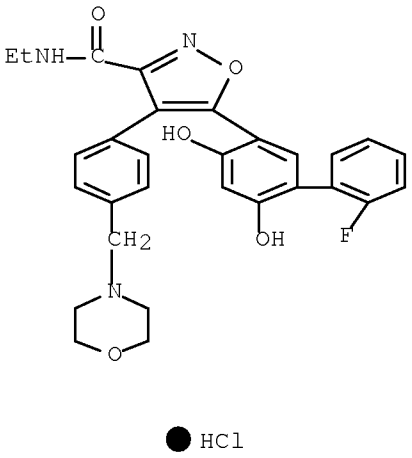
RN 747413-82-7 CAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(1-piperidinylmethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



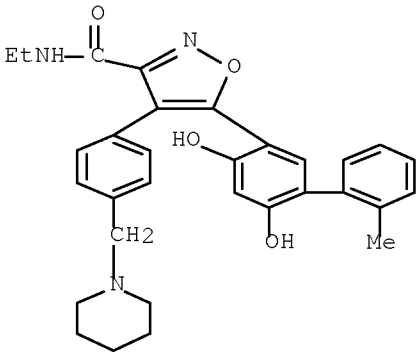
RN 747413-88-3 CAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-(1-piperidinylmethyl)phenyl]- (CA INDEX NAME)



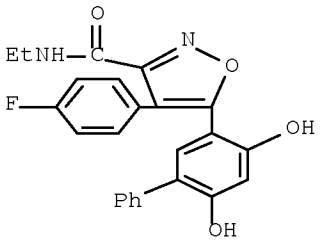
RN 747413-92-9 CAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(2'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(4-morpholinylmethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



RN 747413-98-5 CAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy-2'-methyl[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-(1-piperidinylmethyl)phenyl]- (CA INDEX NAME)



IT 747413-77-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of diphenylisoxazolecarboxamides and diphenylpyrazolecarboxamides as heat shock protein chaperone inhibitors and anticancer agents)
RN 747413-77-0 CAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-(4-fluorophenyl)- (CA INDEX NAME)

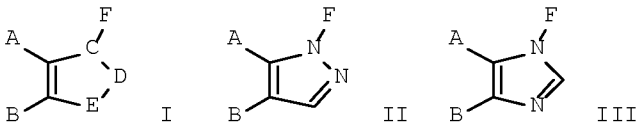


REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

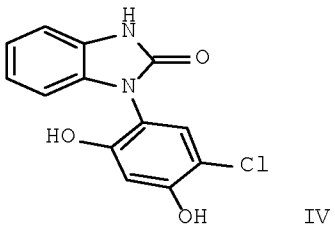
L19 ANSWER 3 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:507527 CAPLUS Full-text
DOCUMENT NUMBER: 146:501047
TITLE: Azole derivatives and related compounds as heat-shock protein binders and inhibitors
INVENTOR(S): Bruncko, Milan; Elmore, Steven W.; Song, Xiaohong; Madar, David J.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 19pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20070105862	A1	20070510	US 2006-593315		20061106
PRIORITY APPLN. INFO.:			US 2005-735716P	P	20051110

OTHER SOURCE(S): MARPAT 146:501047
GI



I II III

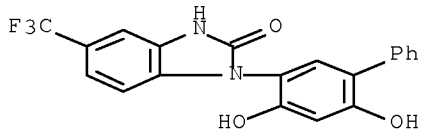


IV

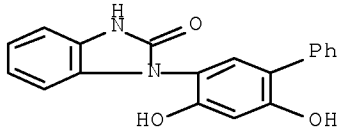
AB Compds. of formula I, II, and III which bind to and inhibit the activity of HSP90, compns. containing the compds. and methods of treating diseases that are caused or exacerbated by overexpression of HSP90 are disclosed. Compds. of formula I, II and III wherein A and B taken together to form benzene; C is CH and N; when D is CH2, CO, NH, O, S, SO, and SO2, E is HC2 and N; when D is CH2 and NH, E is CH2, CO, NH, O, S, SO, and SO2; F is (un)substituted (un)fused 2-hydroxyphenyl; and their therapeutically acceptable salts thereof. Compound IV can be prepared by a generic procedure. The compds. of the invention were evaluated for their heat-shock protein binding and inhibitory activities.

IT 936217-67-3P 936217-71-9P 936217-72-0P
936217-73-1P 936217-74-2P 936217-75-3P
936217-81-1P 936217-82-2P 936217-83-3P
936217-84-4P 936217-85-5P 936217-86-6P
936217-87-7P 936217-88-8P 936217-89-9P
936217-90-2P 936217-91-3P 936217-97-9P
936217-98-0P 936217-99-1P 936218-00-7P
936218-01-8P 936218-02-9P 936218-03-0P
936218-04-1P 936218-05-2P 936218-06-3P
936218-07-4P 936218-08-5P 936218-09-6P
936218-10-9P 936218-11-0P 936218-12-1P
936218-13-2P 936218-18-7P 936218-19-8P
936218-20-1P 936218-21-2P 936218-22-3P
936218-23-4P 936218-29-0P 936218-36-9P
936218-37-0P 936218-38-1P 936218-42-7P
936218-43-8P 936218-44-9P 936218-45-0P
936218-47-2P 936218-61-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azole derivs. and related compds. as HSP90 binders and inhibitors useful in the treatment of diseases caused by or exacerbated by overexpression of HSP90)

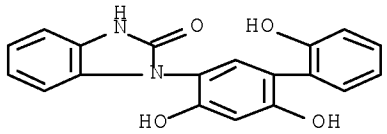
RN 936217-67-3 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



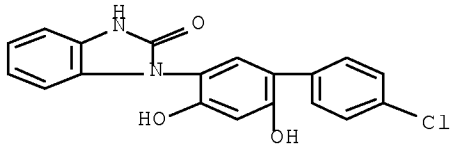
RN 936217-71-9 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



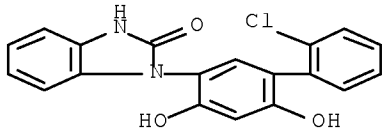
RN 936217-72-0 CAPLUS
CN 2H-Benzimidazol-2-one, 1,3-dihydro-1-(2',4,6-trihydroxy[1,1'-biphenyl]-3-yl)- (CA INDEX NAME)



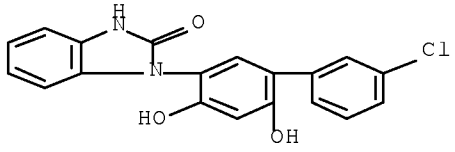
RN 936217-73-1 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4'-chloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



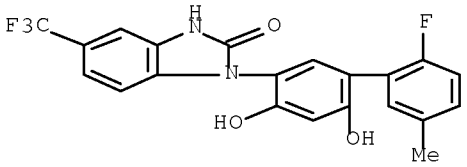
RN 936217-74-2 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(2'-chloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



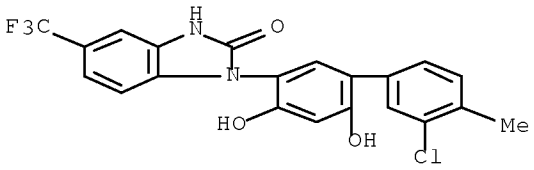
RN 936217-75-3 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(3'-chloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



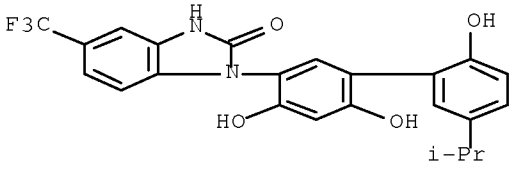
RN 936217-81-1 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(2'-fluoro-4,6-dihydroxy-5'-methyl[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



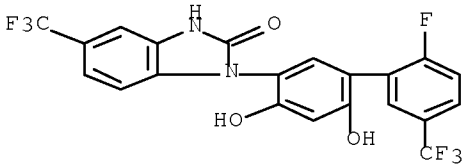
RN 936217-82-2 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(3'-chloro-4,6-dihydroxy-4'-methyl[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



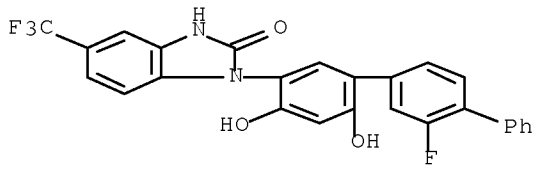
RN 936217-83-3 CAPLUS
CN 2H-Benzimidazol-2-one, 1,3-dihydro-5-(trifluoromethyl)-1-[2',4,6-trihydroxy-5'-(1-methylethyl)[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)



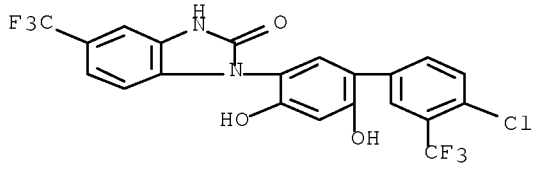
RN 936217-84-4 CAPLUS
CN 2H-Benzimidazol-2-one, 1-[2'-fluoro-4,6-dihydroxy-5'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



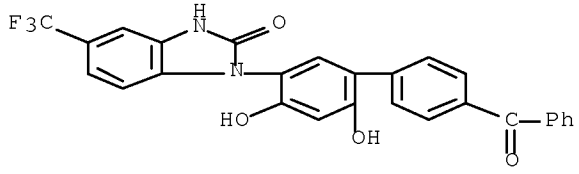
RN 936217-85-5 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(3'-fluoro-4,6-dihydroxy[1,1':4',1''-terphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



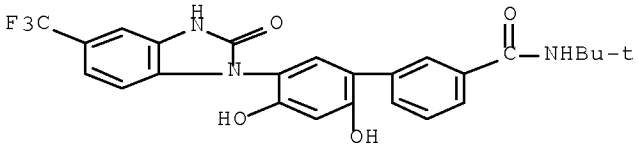
RN 936217-86-6 CAPLUS
CN 2H-Benzimidazol-2-one, 1-[4'-chloro-4,6-dihydroxy-3'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



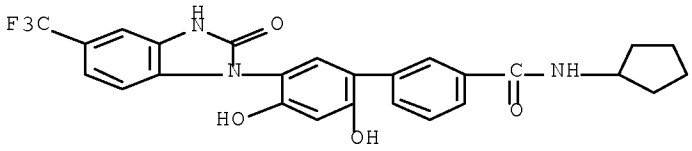
RN 936217-87-7 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4'-benzoyl-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



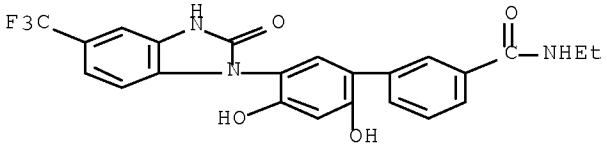
RN 936217-88-8 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 5'-[2,3-dihydro-2-oxo-5-(trifluoromethyl)-1H-benzimidazol-1-yl]-N-(1,1-dimethylethyl)-2',4'-dihydroxy- (CA INDEX NAME)



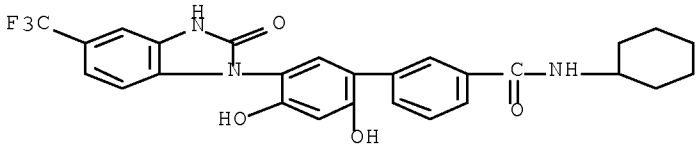
RN 936217-89-9 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, N-cyclopentyl-5'-[2,3-dihydro-2-oxo-5-(trifluoromethyl)-1H-benzimidazol-1-yl]-2',4'-dihydroxy- (CA INDEX NAME)



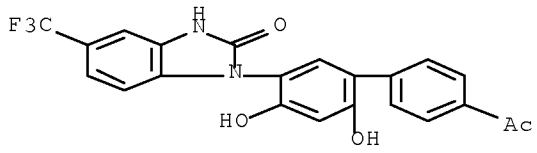
RN 936217-90-2 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 5'-[2,3-dihydro-2-oxo-5-(trifluoromethyl)-1H-benzimidazol-1-yl]-N-ethyl-2',4'-dihydroxy- (CA INDEX NAME)



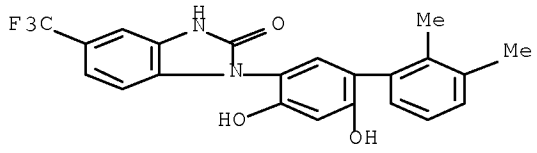
RN 936217-91-3 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, N-cyclohexyl-5'-[2,3-dihydro-2-oxo-5-(trifluoromethyl)-1H-benzimidazol-1-yl]-2',4'-dihydroxy- (CA INDEX NAME)



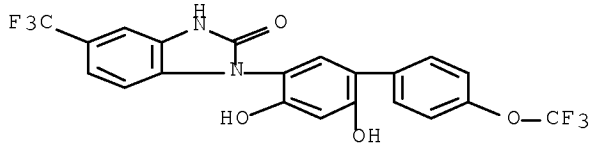
RN 936217-97-9 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4'-acetyl-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



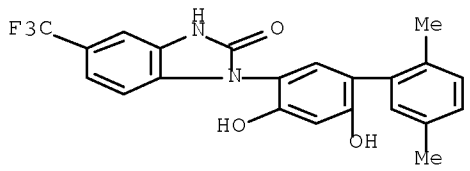
RN 936217-98-0 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy-2',3'-dimethyl[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



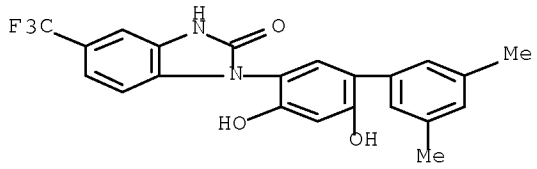
RN 936217-99-1 CAPLUS
CN 2H-Benzimidazol-2-one, 1-[4,6-dihydroxy-4'-(trifluoromethoxy)[1,1'-biphenyl]-3-yl]-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



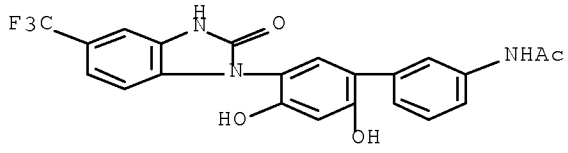
RN 936218-00-7 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy-2',5'-dimethyl[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



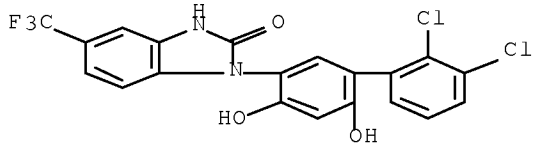
RN 936218-01-8 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy-3',5'-dimethyl[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



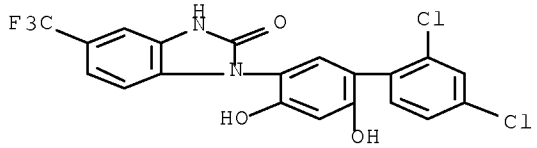
RN 936218-02-9 CAPLUS
CN Acetamide, N-[5'-[2,3-dihydro-2-oxo-5-(trifluoromethyl)-1H-benzimidazol-1-yl]-2',4'-dihydroxy[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)



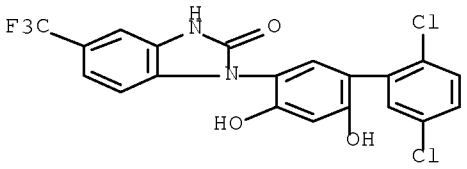
RN 936218-03-0 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(2',3'-dichloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



RN 936218-04-1 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(2',4'-dichloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



RN 936218-05-2 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(2',5'-dichloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



RN 936218-06-3 CAPLUS
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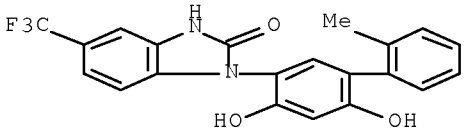

RN 936218-07-4 CAPLUS
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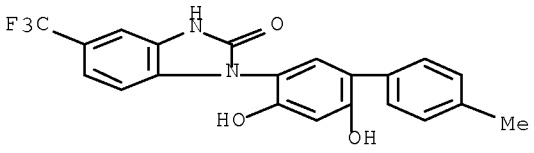

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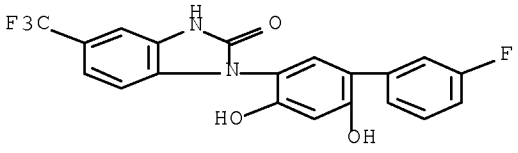
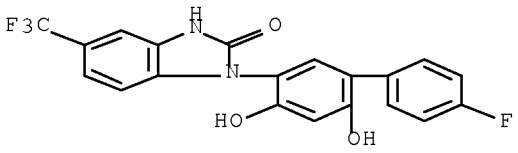
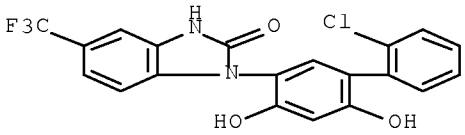


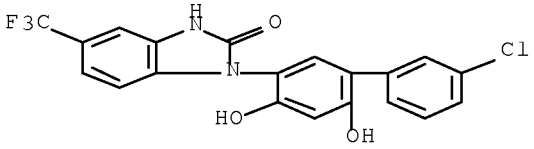
RN 936218-09-6 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



RN 936218-10-9 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(2'-chloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



RN 936218-11-0 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(3'-chloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



RN 936218-12-1 CAPLUS
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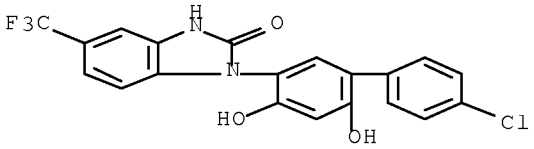

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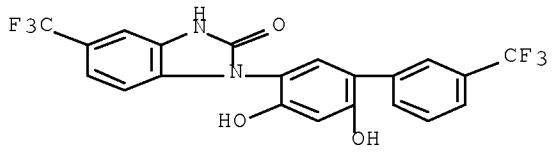
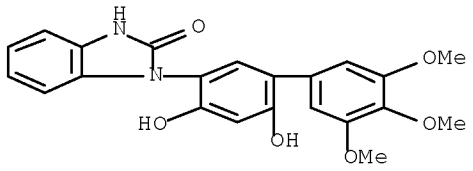
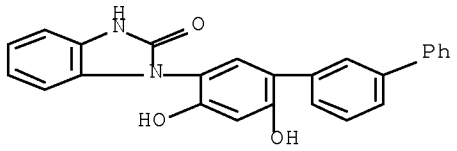


RN 936218-18-7 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy-3',4',5'-trimethoxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



RN 936218-19-8 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy[1,1':3',1''-terphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



RN 936218-20-1 CAPLUS
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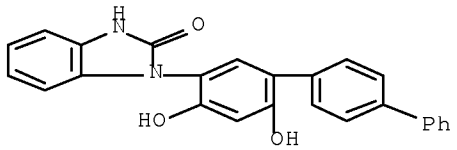
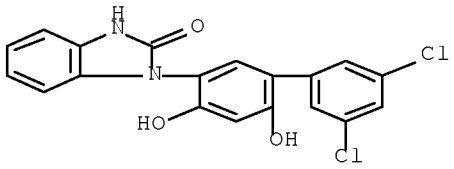
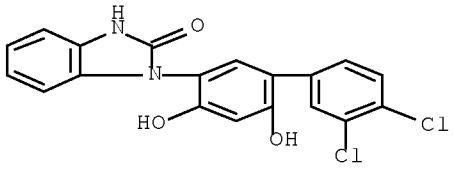


RN 936218-21-2 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(3',5'-dichloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



RN 936218-22-3 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(3',4'-dichloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



RN 936218-23-4 CAPLUS
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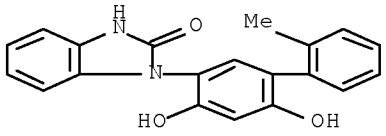
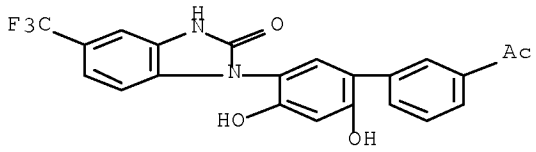
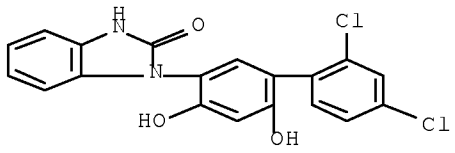


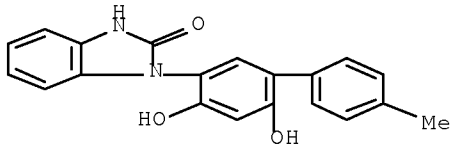
RN 936218-29-0 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(3'-acetyl-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro-5-(trifluoromethyl)- (CA INDEX NAME)



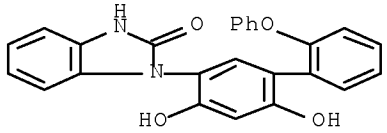
RN 936218-36-9 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(2',4'-dichloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



RN 936218-37-0 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy-4'-methyl[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



RN 936218-38-1 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy-2'-phenoxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



RN 936218-42-7 CAPLUS
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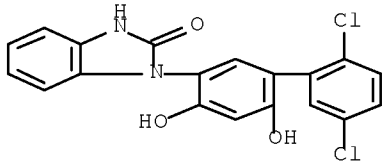
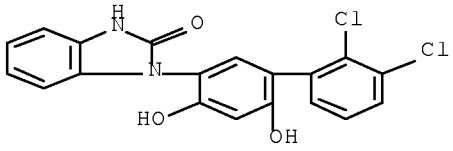
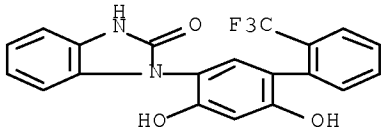


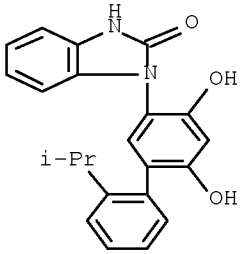
RN 936218-43-8 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(2',3'-dichloro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



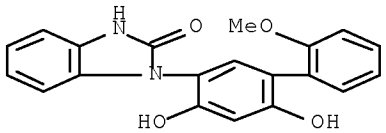
RN 936218-44-9 CAPLUS
CN 2H-Benzimidazol-2-one, 1-[4,6-dihydroxy-2'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-1,3-dihydro- (CA INDEX NAME)



RN 936218-45-0 CAPLUS
CN 2H-Benzimidazol-2-one, 1-[4,6-dihydroxy-2'-(1-methylethyl)[1,1'-biphenyl]-3-yl]-1,3-dihydro- (CA INDEX NAME)



RN 936218-47-2 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(4,6-dihydroxy-2'-methoxy[1,1'-biphenyl]-3-yl)-1,3-dihydro- (CA INDEX NAME)



RN 936218-61-0 CAPLUS
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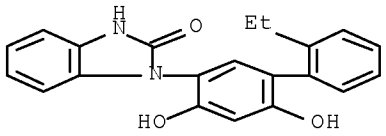
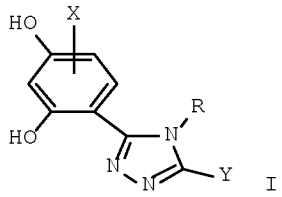


L19 ANSWER 4 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:944485 CAPLUS Full-text
DOCUMENT NUMBER: 145:336056
TITLE: Preparation of 3-(2,4-dihydroxyphenyl)-1,2,4-triazole derivatives as novel inhibitors of heat-shock proteins HSP 90
INVENTOR(S): Kuramochi, Hiroshi; Niitsuma, Setsuko; Nakamura, Masaharu; Sato, Yoshitaka; Saito, Seiichi; Tomura, Arihiro; Ichikawa, Yuh-Ichiro; Kasuga, Yousuke
PATENT ASSIGNEE(S): Nippon Kayaku Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 167pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006095783	A1	20060914	WO 2006-JP304496	20060308
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
CA 2598899	A1	20060914	CA 2006-2598899	20060308
EP 1857446	A1	20071121	EP 2006-715416	20060308
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
KR 2007112400	A	20071123	KR 2007-722889	20071008
CN 101160291	A	20080409	CN 2006-80012406	20071015

PRIORITY APPLN. INFO.:		
JP 2005-65027	A	20050309
JP 2005-183259	A	20050623
WO 2006-JP304496	W	20060308

OTHER SOURCE(S): MARPAT 145:336056
GI



I

AB The title compds. [I; X = SH, HO, halo, NO2, cyano, CO2H, each (un)substituted alkyl, alkenyl, alkynyl, carbocyclic or heterocyclic aryl, alkylthio, arylthio, alkylsulfinyl, arylsulfinyl, alkylsulfonyl, arylsulfonyl, SO2NH2, alkoxyl, aryloxy, acyloxy, alkoxycarbonyloxy, carbamoyloxy, NH2, acylamino, alkoxycarbonylamino, ureido, sulfonylamino, sulfamoylamino, formyl, aryl, alkoxycarbonyl, CONH2, or silyl; Y = SH, HO, halo, cyano, each (un)substituted sulfonyl, alkylthio, arylthio, arylsulfinyl, SO2NH2, alkoxyl, aryloxy, acyloxy, alkoxycarbonyloxy, carbamoyloxy, NH2, acylamino, alkoxycarbonylamino, ureido, sulfonylamino, sulfamoylamino, formyl, acyl, or silyl; R = each (un)substituted carbocyclic or heterocyclic aryl, alkyl, alkenyl, alkynyl, or NH2] or pharmacol. acceptable salts thereof are prepared These compds. inhibit the function of HSP 90 by binding to the ATP-binding site of HSP 90 and thereby inhibit proliferation of cells and are useful as anticancer agents. Thus, 4-[4-(morpholin-4-yl)-phenyl]semicarbazide was condensed with 5-isopropyl-2,4-bis(methoxymethoxy)benzoic acid using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide and HOBt in a mixture of N-methylpyrrolidone and DMF at room temperature overnight to give 70% 4-[4-(morpholin-4-yl)phenyl]-1-[5-isopropyl-2,4- bis(methoxymethoxy)benzoyl]semicarbazide (II). II was cyclized by heating in 5% aqueous NaOH solution at 105° for 2 h and then adding KOH and heating at 130° for 3 h to give 16% 5-[5-isopropyl-2,4-bis(methoxymethoxy)phenyl]-4-[4-(morpholin-4-yl)-phenyl]-4H-[1,2,4]triazol- 3-ol which was treated with a mixture of 5 N aqueous HCl solution and MeOH at room temperature for 4 h to give 4-(5-hydroxy-4-[4-(morpholin-4-yl)phenyl]-4H-[1,2,4]triazol-3-yl)-6-isopropylbenzene-1,3-diol (III). III in vitro showed IC50 of μg/mL against HSP 90 in an assay inducing the reduction of HSP 90-binding proteins Her and ERα in MCF7 cells and in vivo showed IC50 of 0.014 μM against human lung cancer in mice.

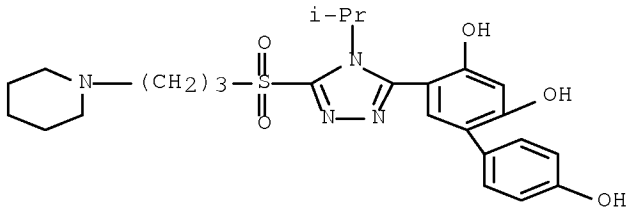
IT 909872-76-0P, 4-(4-Hydroxyphenyl)-6-[4-isopropyl-5-[[3-(piperidin-1-yl)propan-1-yl]sulfonyl]-4H-1,2,4-triazol-3-yl]benzene-1,3-diol monotrifluoroacetate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3-(2,4-dihydroxyphenyl)-1,2,4-triazole derivs. as inhibitors of heat-shock proteins HSP 90 and anticancer agents)

RN 909872-76-0 CAPLUS

CN [1,1'-Biphenyl]-2,4,4'-triol, 5-[4-(1-methylethyl)-5-[[3-(1-piperidinyl)propyl]sulfonyl]-4H-1,2,4-triazol-3-yl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

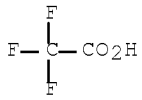
CM 1

CRN 909872-75-9
CMF C25 H32 N4 O5 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:431871 CAPLUS Full-text
DOCUMENT NUMBER: 145:124995
TITLE: Oligoresorcinols Fold into Double Helices in Water
AUTHOR(S): Goto, Hidetoshi; Katagiri, Hiroshi; Furusho, Yoshio; Yashima, Eiji
CORPORATE SOURCE: Yashima Super-structured Helix Project ERATO, Japan Science and Technology Agency (JST), 2266-22 Shimoshidami, Moriyama-ku, Nagoya, 463-0003, Japan
SOURCE: Journal of the American Chemical Society (2006), 128(22), 7176-7178
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:124995

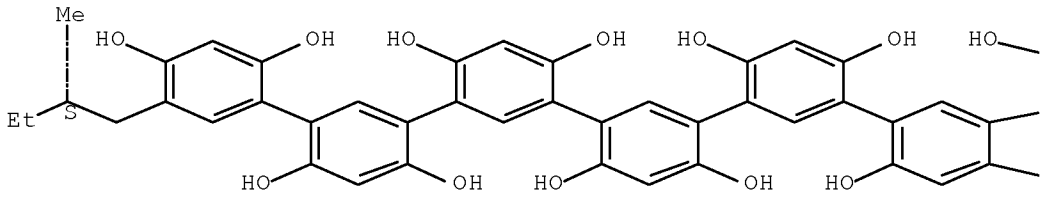
AB We report the first double helixes with a controlled helicity in water based on oligoresorcinols as a new, simplest water-soluble structural motif. The mol. strands of the oligoresorcinols self-assemble into double helixes with the aid of aromatic interactions in water as characterized by 1H NMR and absorption spectroscopies together with the X-ray crystallog. study of the pentamer. The double helix formation is sensitive to the chain length, solvent composition, and temperature Moreover, a bias in the screw sense of the double helixes was achieved by covalently attaching chiral substituents to both ends of the mol. strands.

IT 896507-46-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and characterization of oligoresorcinols capable of folding into double helixes in water)
RN 896507-46-3 CAPLUS

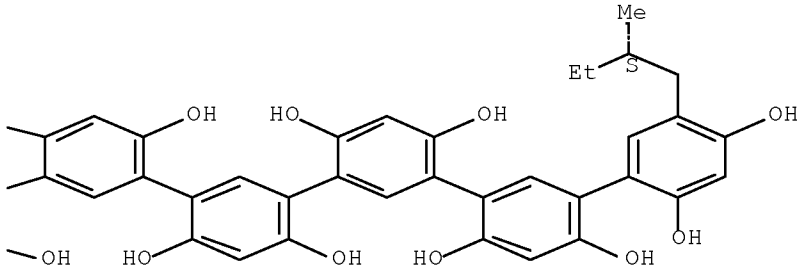
CN [1,1':3',1'':3'',1''':3''',1'''':3'''',1''''':3''''',1'''''':3'''''',1''''''':3''''''',1'''''''':3'''''''',1'''''''''':3'''''''',1''''''''':3''''''''',1'''''''''':3''''''''',1''''''''''-Undeciphenyl]-2,2''''''''''',4,4',4'',4''',4'''',4''''',4'''''',4''''''',4'''''''',4''''''''',4''''''''',6',6'',6''',6'''',6''''',6'''''',6''''''',6'''''''',6''''''''',6'''''''''-docosaol, 5,5''''''''''-bis[(2S)-2-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

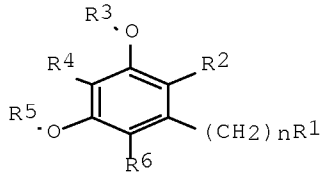
L19 ANSWER 6 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:612072 CAPLUS Full-text
DOCUMENT NUMBER: 143:146661
TITLE: Hsp90 family protein inhibitor
INVENTOR(S): Kitamura, Yushi; Nara, Shinji; Nakagawa, Hiroshi; Nakatsu, Rieko; Nakashima, Takayuki; Soga, Shiro; Kajita, Jiro; Shiotsu, Yukimasa; Kanda, Yutaka
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: PCT Int. Appl., 311 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2005063222	A1	20050714	WO 2004-JP19742	20041224
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1704856	A1	20060927	EP 2004-808092	20041224
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
US 20070155813	A1	20070705	US 2006-584234	20060626
PRIORITY APPLN. INFO.:			JP 2003-432776 A	20031226
			WO 2004-JP19742 W	20041224

OTHER SOURCE(S): MARPAT 143:146661

GI



I

AB A Hsp90 family protein inhibitor which contains as an active ingredient a benzene derivative represented by the following general formula (I), a prodrug thereof, or a pharmacol. acceptable salt of either.

IT 860151-78-6P 860151-80-0P 860151-83-3P
860151-86-6P 860151-87-7P 860151-88-8P
860151-90-2P 860151-92-4P 860151-94-6P
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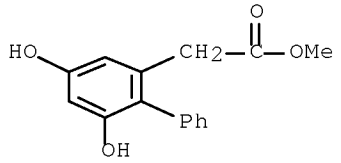
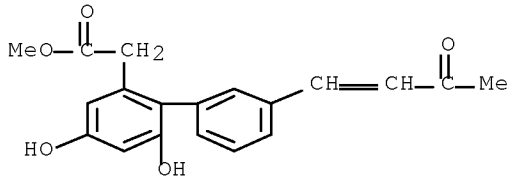
860293-46-5P 860293-47-6P 860293-48-7P
860293-62-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(benzene derivs. as Hsp90 family protein inhibitors and antitumor agents)

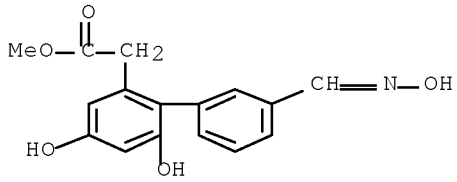
RN 860151-78-6 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-, methyl ester (CA INDEX NAME)



RN 860151-80-0 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-(3-oxo-1-buten-1-yl)-, methyl ester (CA INDEX NAME)



RN 860151-83-3 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-[(hydroxyimino)methyl]-, methyl ester (CA INDEX NAME)



RN 860151-86-6 CAPLUS
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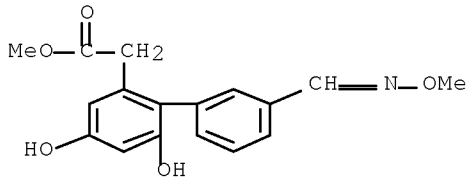
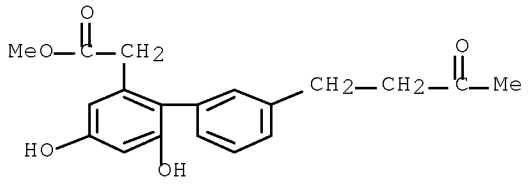
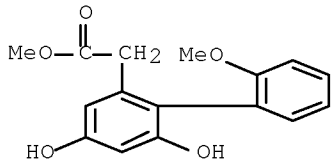


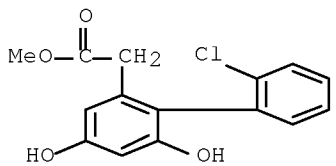
RN 860151-87-7 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-(3-oxobutyl)-, methyl ester (CA INDEX NAME)



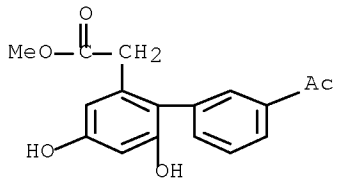
RN 860151-88-8 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-2'-methoxy-, methyl ester (CA INDEX NAME)



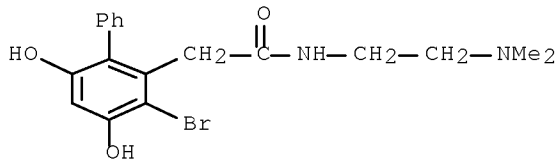
RN 860151-90-2 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 2'-chloro-4,6-dihydroxy-, methyl ester (CA INDEX NAME)



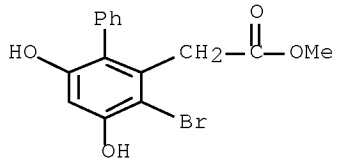
RN 860151-92-4 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 3'-acetyl-4,6-dihydroxy-, methyl ester (CA INDEX NAME)



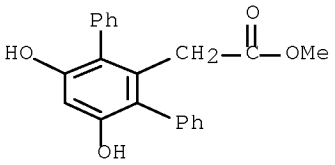
RN 860151-94-6 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-N-[2-(dimethylamino)ethyl]-4,6-dihydroxy- (CA INDEX NAME)



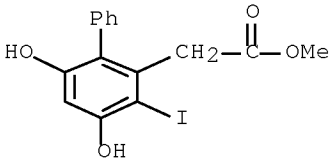
RN 860151-96-8 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 3-bromo-4,6-dihydroxy-, methyl ester (CA INDEX NAME)



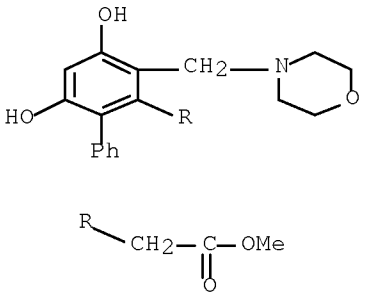
RN 860151-98-0 CAPLUS
CN [1,1':3',1''-Terphenyl]-2'-acetic acid, 4',6'-dihydroxy-, methyl ester (9CI) (CA INDEX NAME)



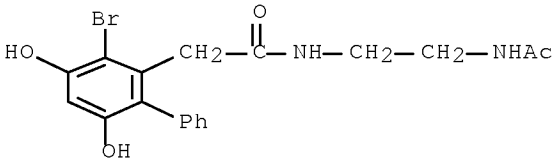
RN 860152-01-8 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3-iodo-, methyl ester (CA INDEX NAME)



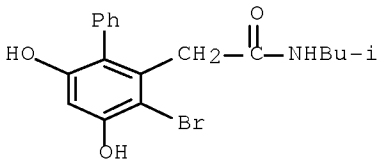
RN 860152-03-0 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3-(4-morpholinylmethyl)-, methyl ester (CA INDEX NAME)



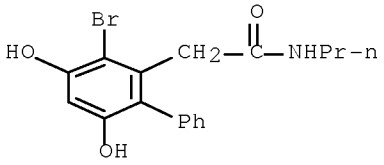
RN 860152-05-2 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, N-[2-(acetylamino)ethyl]-3-bromo-4,6-dihydroxy- (CA INDEX NAME)



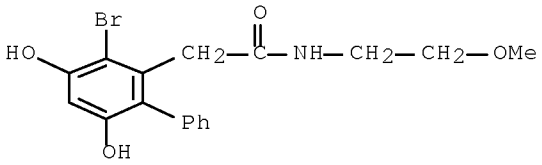
RN 860152-09-6 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(2-methylpropyl)- (CA INDEX NAME)



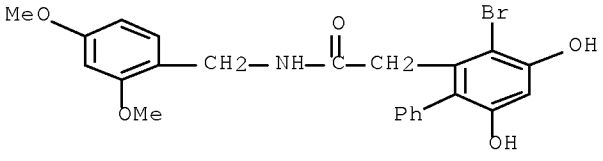
RN 860152-10-9 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-propyl- (CA INDEX NAME)



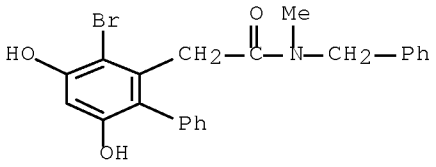
RN 860152-12-1 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(2-methoxyethyl)- (CA INDEX NAME)



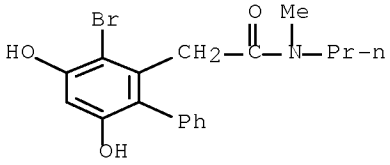
RN 860152-17-6 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-N-[(2,4-dimethoxyphenyl)methyl]-4,6-dihydroxy- (CA INDEX NAME)



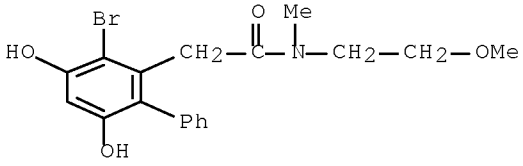
RN 860152-18-7 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-methyl-N-(phenylmethyl)- (CA INDEX NAME)



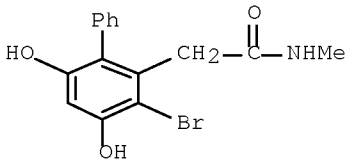
RN 860152-25-6 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-methyl-N-propyl- (CA INDEX NAME)



RN 860152-26-7 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-(2-methoxyethyl)-N-methyl- (CA INDEX NAME)



RN 860152-30-3 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-methyl- (CA INDEX NAME)



RN 860152-31-4 CAPLUS
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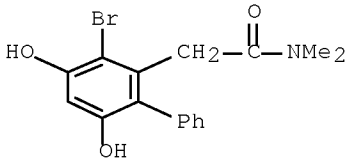
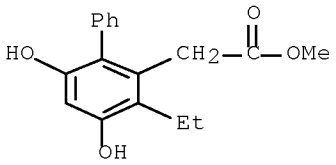
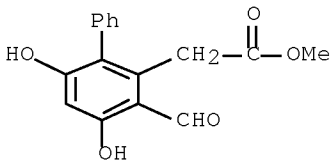


RN 860152-40-5 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 3-ethyl-4,6-dihydroxy-, methyl ester (CA INDEX NAME)



RN 860152-43-8 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 3-formyl-4,6-dihydroxy-, methyl ester (CA INDEX NAME)



RN 860152-44-9 CAPLUS
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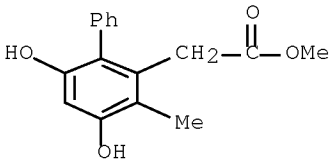

RN 860152-54-1 CAPLUS
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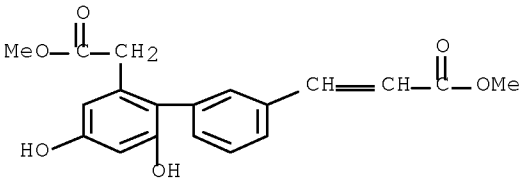
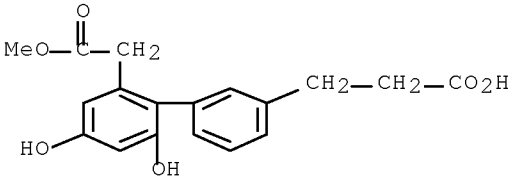


RN 860152-55-2 CAPLUS
CN [1,1'-Biphenyl]-3-propanoic acid, 2',4'-dihydroxy-6'-(2-methoxy-2-oxoethyl)- (CA INDEX NAME)



RN 860152-56-3 CAPLUS
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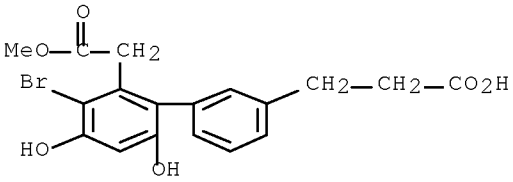

RN 860152-57-4 CAPLUS

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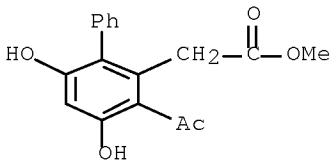
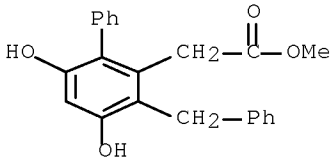
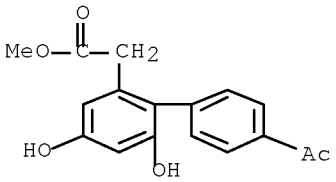


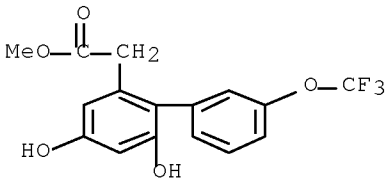
RN 860152-58-5 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3-(phenylmethyl)-, methyl ester (CA INDEX NAME)



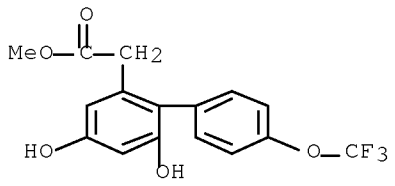
RN 860152-61-0 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4'-acetyl-4,6-dihydroxy-, methyl ester (CA INDEX NAME)



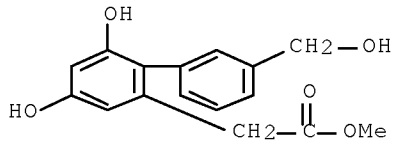
RN 860152-62-1 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-(trifluoromethoxy)-, methyl ester (CA INDEX NAME)



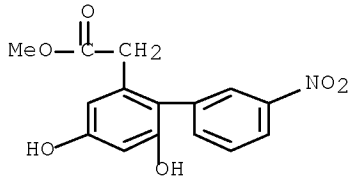
RN 860152-63-2 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-4'-(trifluoromethoxy)-, methyl ester (CA INDEX NAME)



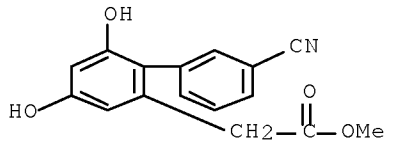
RN 860152-64-3 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-(hydroxymethyl)-, methyl ester (CA INDEX NAME)



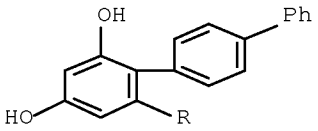
RN 860152-65-4 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-nitro-, methyl ester (CA INDEX NAME)

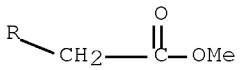


RN 860152-66-5 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 3'-cyano-4,6-dihydroxy-, methyl ester (CA INDEX NAME)

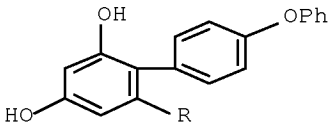


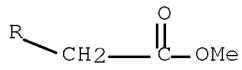
RN 860152-67-6 CAPLUS
CN [1,1':4',1''-Terphenyl]-2-acetic acid, 4,6-dihydroxy-, methyl ester (9CI) (CA INDEX NAME)



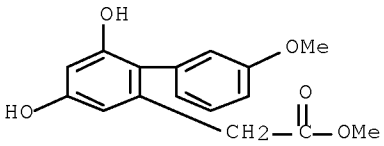


RN 860152-68-7 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-4'-phenoxy-, methyl ester (CA INDEX NAME)

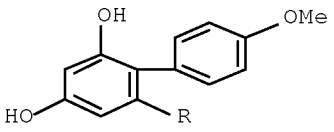


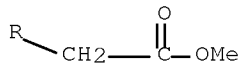


RN 860152-69-8 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-3'-methoxy-, methyl ester (CA INDEX NAME)

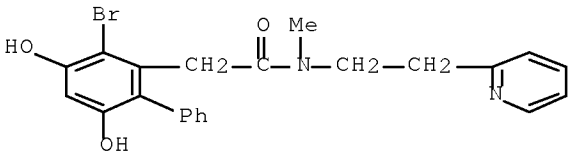


RN 860152-70-1 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 4,6-dihydroxy-4'-methoxy-, methyl ester (CA INDEX NAME)

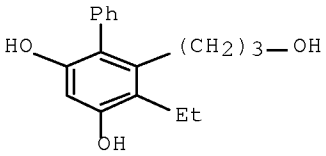




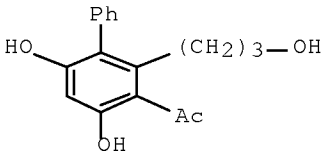
RN 860152-77-8 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-bromo-4,6-dihydroxy-N-methyl-N-[2-(2-pyridinyl)ethyl]- (CA INDEX NAME)



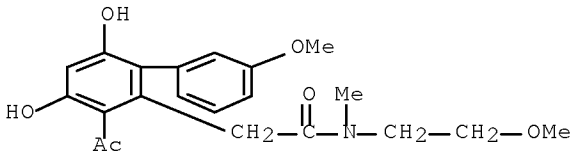
RN 860153-11-3 CAPLUS
CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-(3-hydroxypropyl)- (CA INDEX NAME)



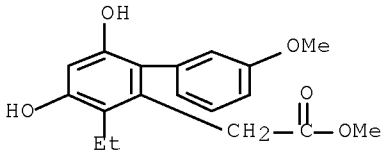
RN 860153-12-4 CAPLUS
CN Ethanone, 1-[4,6-dihydroxy-2-(3-hydroxypropyl)[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)



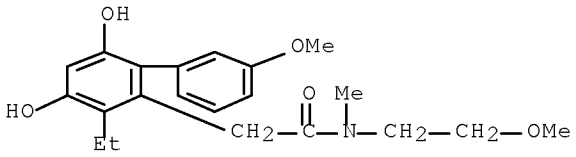
RN 860153-29-3 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-acetyl-4,6-dihydroxy-3'-methoxy-N-(2-methoxyethyl)-N-methyl- (CA INDEX NAME)



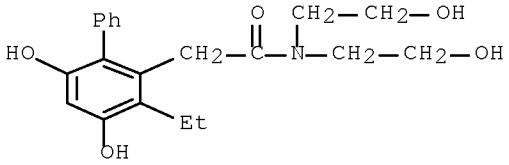
RN 860153-30-6 CAPLUS
CN [1,1'-Biphenyl]-2-acetic acid, 3-ethyl-4,6-dihydroxy-3'-methoxy-, methyl ester (CA INDEX NAME)



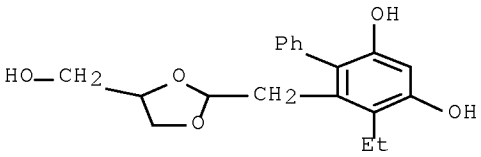
RN 860153-38-4 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-ethyl-4,6-dihydroxy-3'-methoxy-N-(2-methoxyethyl)-N-methyl- (CA INDEX NAME)



RN 860153-86-2 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-ethyl-4,6-dihydroxy-N,N-bis(2-hydroxyethyl)- (CA INDEX NAME)

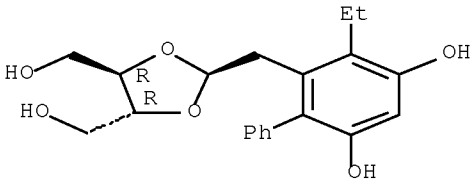


RN 860153-99-7 CAPLUS
CN [1,1'-Biphenyl]-2,4-diol, 5-ethyl-6-[[4-(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]- (CA INDEX NAME)



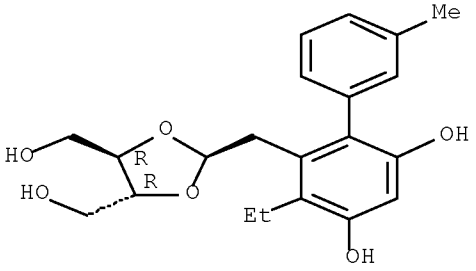
RN 860154-06-9 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



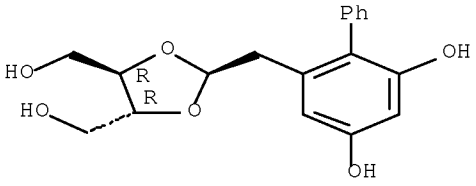
RN 860154-15-0 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy-3'-methyl[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



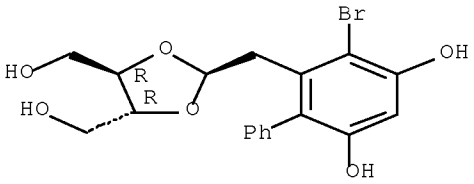
RN 860154-16-1 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



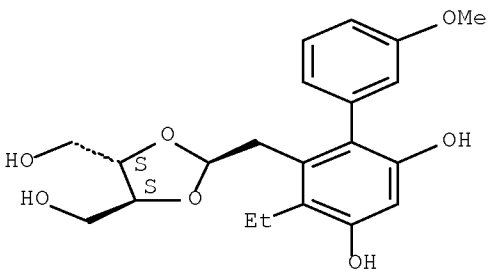
RN 860154-18-3 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-bromo-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



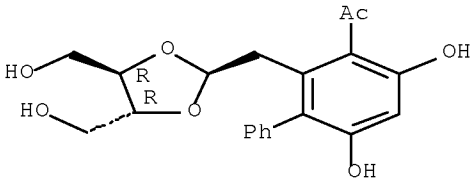
RN 860154-19-4 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy-3'-methoxy[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



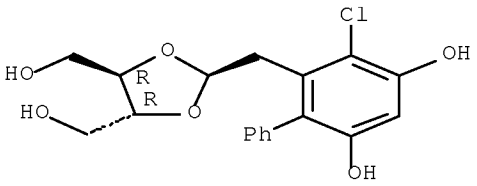
RN 860154-20-7 CAPLUS
CN Ethanone, 1-[2-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-4,6-dihydroxy[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.



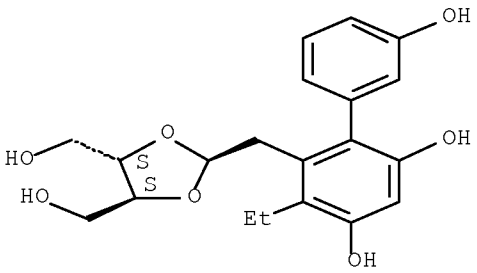
RN 860154-66-1 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-chloro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



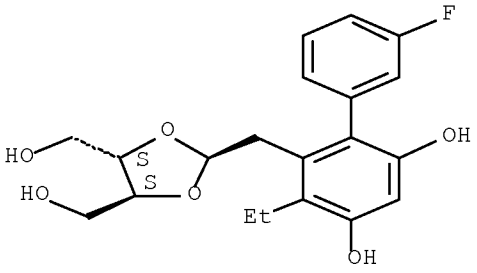
RN 860154-67-2 CAPLUS
CN [1,1'-Biphenyl]-2,3',4-triol, 6-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-5-ethyl- (CA INDEX NAME)

Absolute stereochemistry.



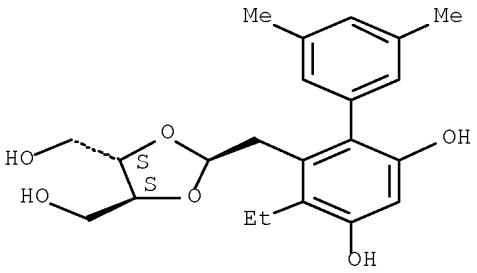
RN 860154-68-3 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-3'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



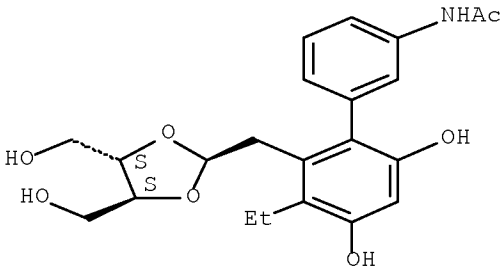
RN 860154-69-4 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy-3',5'-dimethyl[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



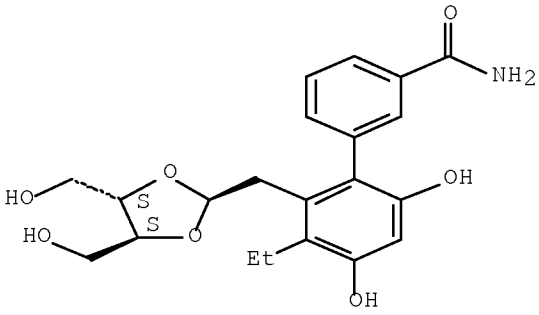
RN 860154-70-7 CAPLUS
CN Acetamide, N-[2'-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.



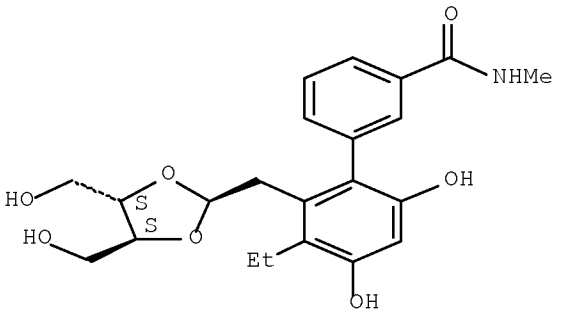
RN 860154-71-8 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy- (CA INDEX NAME)

Absolute stereochemistry.



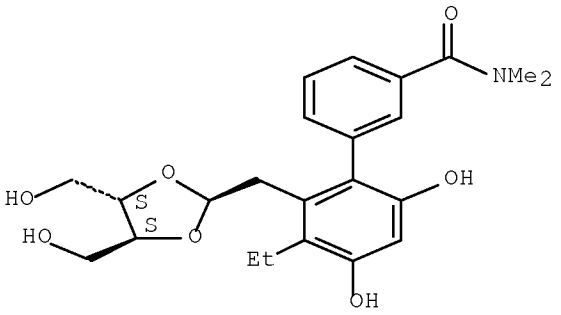
RN 860154-72-9 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



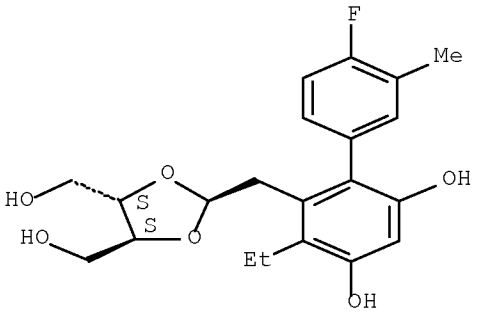
RN 860154-73-0 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N,N-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.



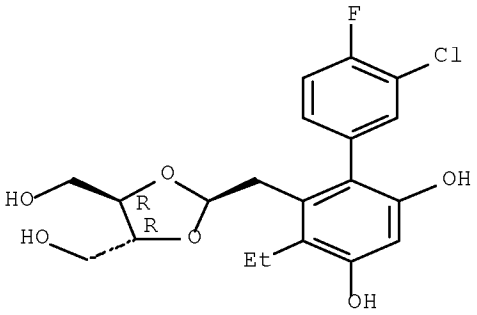
RN 860154-74-1 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4'-fluoro-4,6-dihydroxy-3'-methyl[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



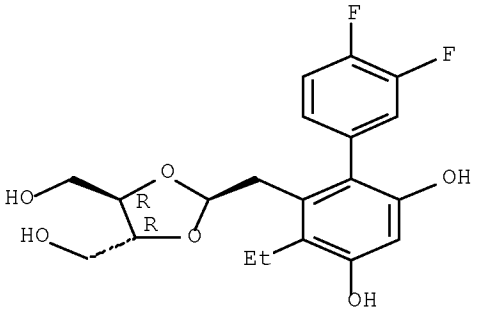
RN 860154-75-2 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3'-chloro-3-ethyl-4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



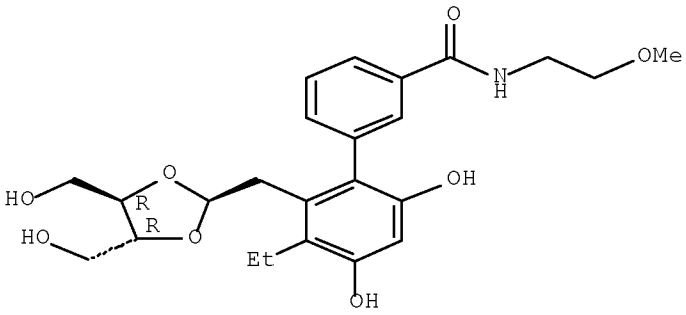
RN 860154-76-3 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-3',4'-difluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



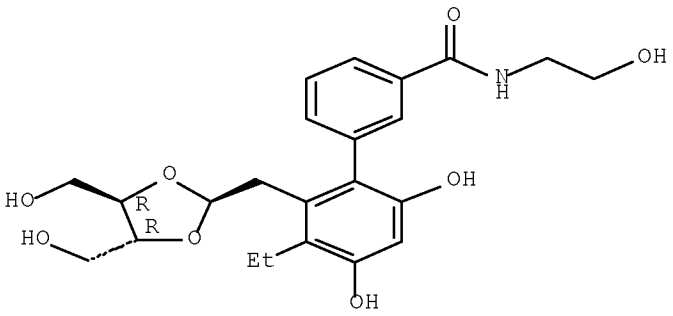
RN 860154-77-4 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-(2-methoxyethyl)- (CA INDEX NAME)

Absolute stereochemistry.



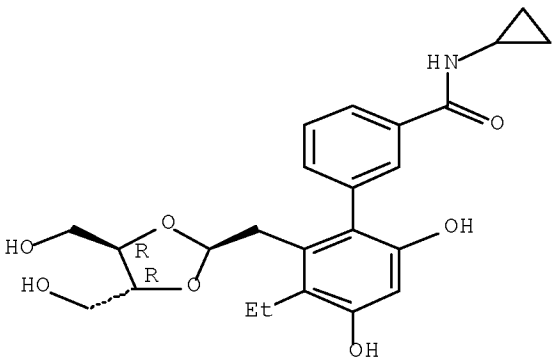
RN 860154-78-5 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-(2-hydroxyethyl)- (CA INDEX NAME)

Absolute stereochemistry.



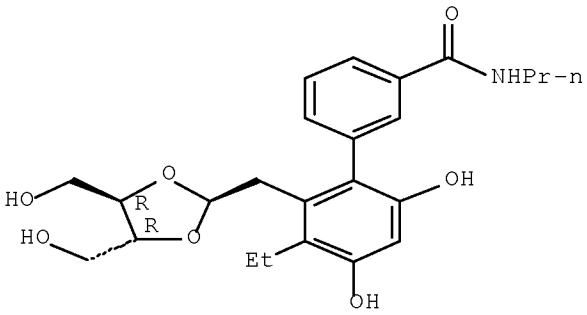
RN 860154-79-6 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-N-cyclopropyl-3'-ethyl-4',6'-dihydroxy- (CA INDEX NAME)

Absolute stereochemistry.



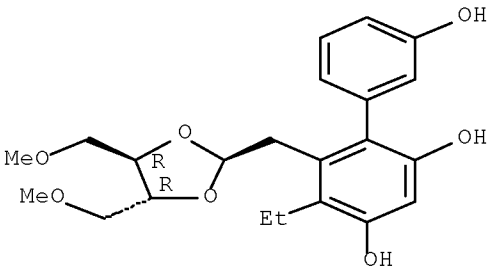
RN 860154-80-9 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-propyl- (CA INDEX NAME)

Absolute stereochemistry.



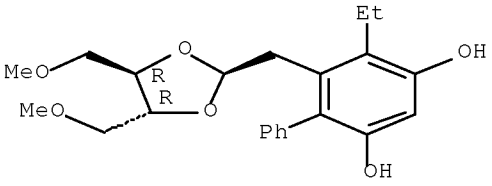
RN 860154-81-0 CAPLUS
CN [1,1'-Biphenyl]-2,3',4-triol, 6-[[(4R,5R)-4,5-bis(methoxymethyl)-1,3-dioxolan-2-yl]methyl]-5-ethyl- (CA INDEX NAME)

Absolute stereochemistry.

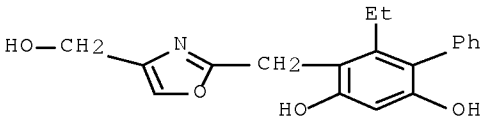


RN 860154-82-1 CAPLUS
CN [1,1'-Biphenyl]-2,4-diol, 6-[[(4R,5R)-4,5-bis(methoxymethyl)-1,3-dioxolan-2-yl]methyl]-5-ethyl- (CA INDEX NAME)

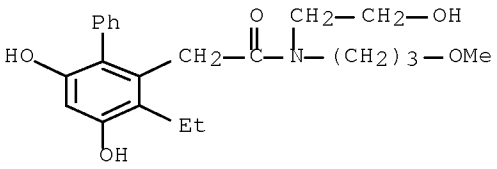
Absolute stereochemistry.



RN 860154-92-3 CAPLUS
CN [1,1'-Biphenyl]-2,4-diol, 6-ethyl-5-[[4-(hydroxymethyl)-2-oxazolyl]methyl]- (CA INDEX NAME)

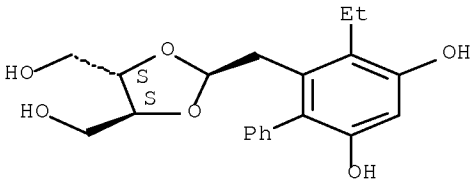


RN 860154-94-5 CAPLUS
CN [1,1'-Biphenyl]-2-acetamide, 3-ethyl-4,6-dihydroxy-N-(2-hydroxyethyl)-N-(3-methoxypropyl)- (CA INDEX NAME)



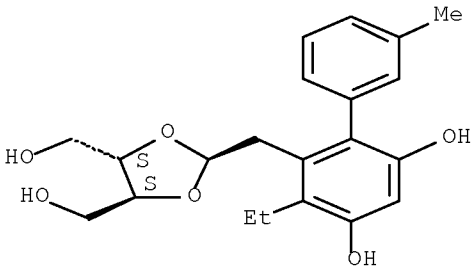
RN 860293-36-3 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



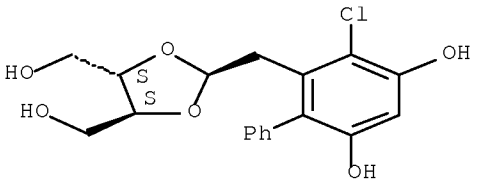
RN 860293-37-4 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy-3'-methyl[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



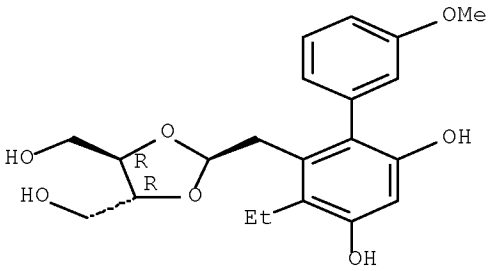
RN 860293-38-5 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-chloro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



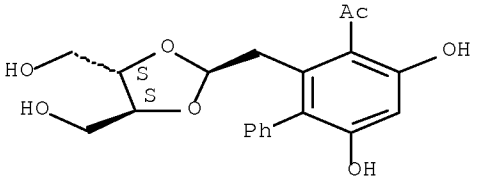
RN 860293-39-6 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy-3'-methoxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



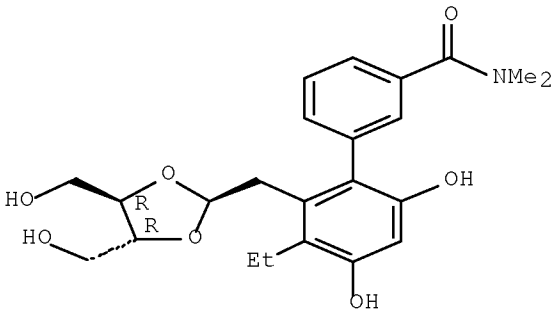
RN 860293-40-9 CAPLUS
CN Ethanone, 1-[2-[[(4S,5S)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-4,6-dihydroxy[1,1'-biphenyl]-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.



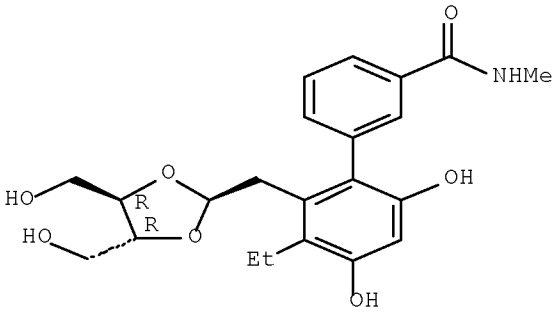
RN 860293-41-0 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N,N-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.



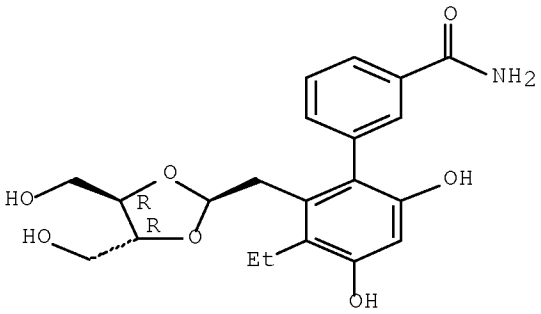
RN 860293-42-1 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



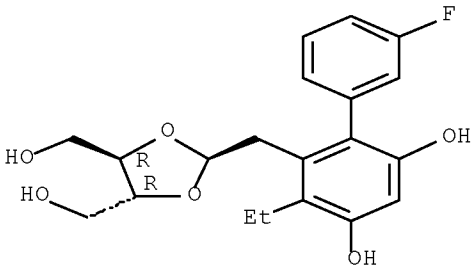
RN 860293-43-2 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, 2'-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-3'-ethyl-4',6'-dihydroxy- (CA INDEX NAME)

Absolute stereochemistry.



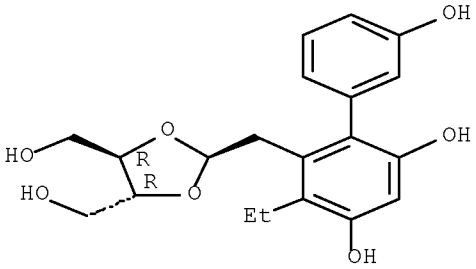
RN 860293-44-3 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-3'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



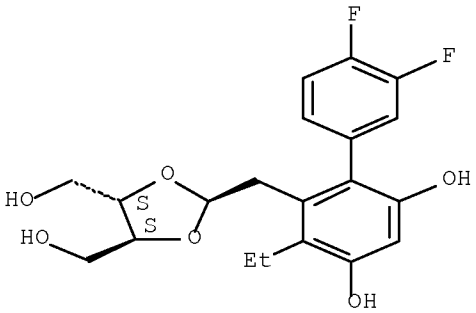
RN 860293-45-4 CAPLUS
CN [1,1'-Biphenyl]-2,3',4-triol, 6-[[(4R,5R)-4,5-bis(hydroxymethyl)-1,3-dioxolan-2-yl]methyl]-5-ethyl- (CA INDEX NAME)

Absolute stereochemistry.



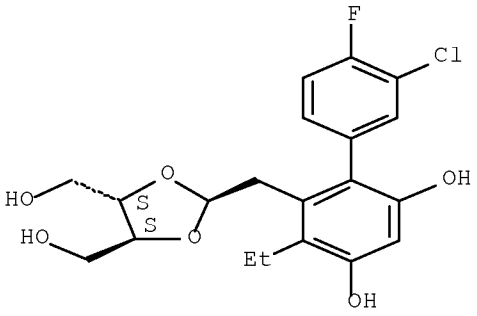
RN 860293-46-5 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-3',4'-difluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



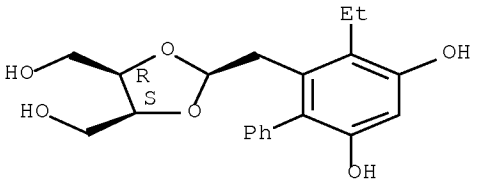
RN 860293-47-6 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3'-chloro-3-ethyl-4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



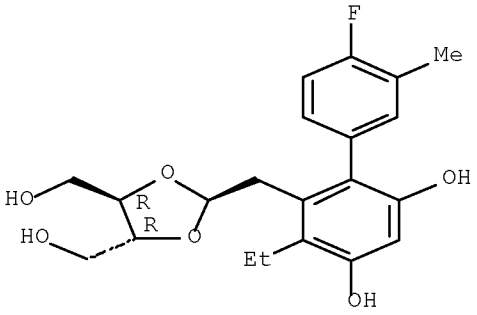
RN 860293-48-7 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



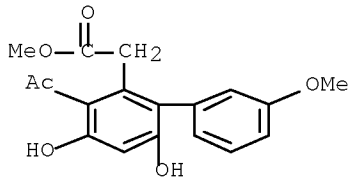
RN 860293-62-5 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(3-ethyl-4'-fluoro-4,6-dihydroxy-3'-methyl[1,1'-biphenyl]-2-yl)methyl]-, (4R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



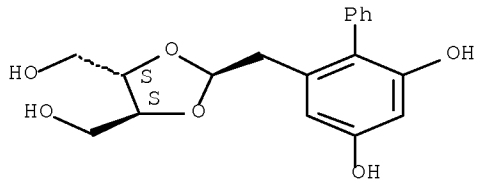
IT 860156-57-6P 860293-52-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(benzene derivs. as Hsp90 family protein inhibitors and antitumor agents)
RN 860156-57-6 CAPLUS

CN [1,1'-Biphenyl]-2-acetic acid, 3-acetyl-4,6-dihydroxy-3'-methoxy-, methyl ester (CA INDEX NAME)



RN 860293-52-3 CAPLUS
CN 1,3-Dioxolane-4,5-dimethanol, 2-[(4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]-, (4S,5S)- (CA INDEX NAME)

Absolute stereochemistry.

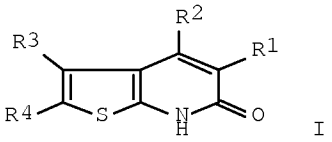


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 7 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:140804 CAPLUS Full-text
DOCUMENT NUMBER: 142:240419
TITLE: Preparation of substituted thieno[2,3-b]pyridones as activators for AMP-activated kinase for the treatment of diabetes and obesity
INVENTOR(S): Iyengar, Rajesh R.; Judd, Andrew S.; Zhao, Gang; Kym, Philip R.; Sham, Hing L.; Gu, Yugui; Liu, Gang; Liu, Mei; Zhao, Hongyu; Clark, Richard F.; Frevert, Ernst U.; Cool, Barbara L.; Zhang, Tianyuan; Keyes, Robert F.; Hansen, Todd M.; Xin, Zhili
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S. Pat. Appl. Publ., 86 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20050038068	A1	20050217	US 2004-847144		20040517
US 7119205	B2	20061010			
US 20060287356	A1	20061221	US 2006-509383		20060824
PRIORITY APPLN. INFO.:			US 2003-471064P	P	20030516
			US 2004-847144	A3	20040517

OTHER SOURCE(S): CASREACT 142:240419; MARPAT 142:240419
GI



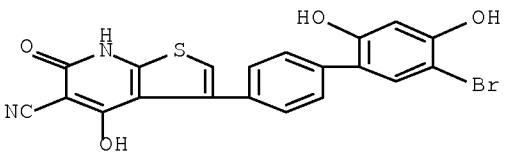
I

AB Title compds. I [R1 = H, alkoxy, alkoxycarbonyl, etc.; R2 = alkoxy, OH, thioalkoxy, etc.; R3 = alkoxycarbonyl, aryl, etc.; R4 = H, alk(en/yn)yl, aryl, etc.] are prepared For instance, 3-(3,5-dimethylphenyl)-4-hydroxy-6- oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile is prepared in several steps from 3,5-dimethylacetophenone, Et cyanoacetate and cyanoacetic acid. Representative compds. of the invention activate AMPK at a dose of 1-100 μM. I are useful for the treatment of disorders such as diabetes, metabolic syndrome and obesity.

IT 844501-31-1P, 3-[4-(5-Bromo-2,4-dihydroxyphenyl)phenyl]-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted thieno[2,3-b]pyridones as activators for AMP-activated kinase for treatment of diabetes and obesity)

RN 844501-31-1 CAPLUS

CN Thieno[2,3-b]pyridine-5-carbonitrile, 3-(5'-bromo-2',4'-dihydroxy[1,1'-biphenyl]-4-yl)-6,7-dihydro-4-hydroxy-6-oxo- (CA INDEX NAME)



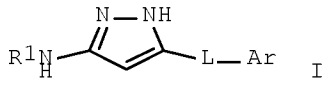
L19 ANSWER 8 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:99354 CAPLUS Full-text
DOCUMENT NUMBER: 142:198068
TITLE: Preparation of aminopyrazoles as CHK1 checkpoint protein kinase inhibitors.
INVENTOR(S): Johnson, Michael David; Teng, Min; Zhu, Jinjiang
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: PCT Int. Appl., 127 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

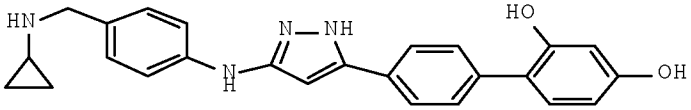
WO 2005009435	A1	20050203	WO 2004-IB2397	20040714
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2532231	A1	20050203	CA 2004-2532231	20040714
BR 2004012820	A	20060926	BR 2004-12820	20040714
JP 2006528661	T	20061221	JP 2006-521691	20040714
US 20050043381	A1	20050224	US 2004-897849	20040722
MX 2006PA00933	A	20060330	MX 2006-PA933	20060124
PRIORITY APPLN. INFO.:			US 2003-489976P P	20030725
			WO 2004-IB2397 W	20040714

OTHER SOURCE(S): CASREACT 142:198068; MARPAT 142:198068

GI



I



II

AB Title compds. [I; L = 5-6 membered (substituted) heterocyclylene; Ar = 5-6 membered (substituted) (hetero)aryl; R1 = (substituted) aryl(alkyl), heterocyclyl(alkyl), cycloalkyl(alkyl), alkenyl, alkyl; R2 = H, halo, (substituted) alkyl], were prepared Thus, title compound (II) (preparation outlined) inhibited human CHK1 with Ki <1 nM.

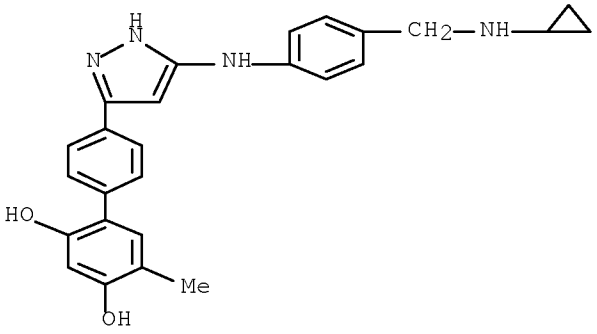
IT 838823-35-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

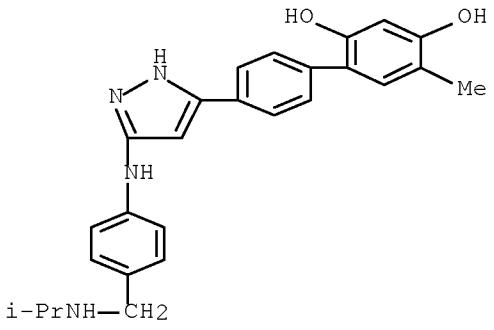
(claimed compound; preparation of aminopyrazoles as CHK1 checkpoint protein kinase inhibitors)

RN 838823-35-1 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 4'-[5-[[4-[(cyclopropylamino)methyl]phenyl]amino]-1H-pyrazol-3-yl]-5-methyl- (CA INDEX NAME)



IT 838824-27-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminopyrazoles as CHK1 checkpoint protein kinase inhibitors)
RN 838824-27-4 CAPLUS
CN [1,1'-Biphenyl]-2,4-diol, 5-methyl-4'-[3-[[4-[[(1-methylethyl)amino]methyl]phenyl]amino]-1H-pyrazol-5-yl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 9 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:788103 CAPLUS Full-text
DOCUMENT NUMBER: 142:170224
TITLE: De Novo ligand design of selective estrogen receptor modulators (SERMs)
AUTHOR(S): Joomprabutra, Surachai
CORPORATE SOURCE: Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmaceutical Sciences, Ubon Ratchathani University, Ubon Rathathani, 34190, Thailand
SOURCE: Warasan Phesatchasat (2003), 30(3), 47-56
CODEN: VPSADN; ISSN: 0125-1570
PUBLISHER: Mahidol University, Faculty of Pharmacy
DOCUMENT TYPE: Journal
LANGUAGE: English

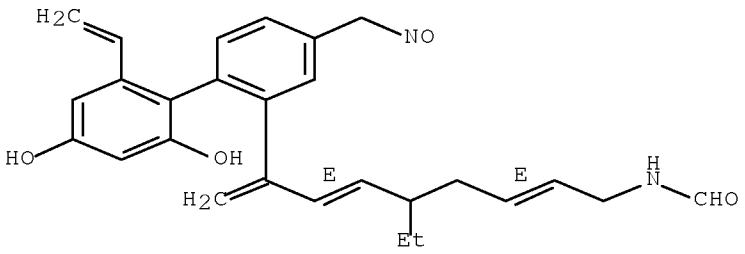
AB Estrogen controls various physiol. processes such as sexual differentiation and development, cardiovascular system, and bone health. The reduction of estrogen in the body like in postmenopausal women leads to an incidence of coronary heart disease and lost of bone mineral d. However, estrogen use in hormone replacement therapy is associated with an increased risk of uterine and breast cancer which limits its use as a replacement in postmenopausal women. The finding of group of estrogen receptor ligands having ability to behave as partial or full agonists in some tissues while behaving as antagonists in others, they are called selective estrogen receptor modulators (SERMs). In this study, preliminary SERMs pharmacophore was developed based on the different in mode of binding of ligands. This pharmacophore was used in the De Novo ligand design process to generate the candidates. Candidates were first evaluated by their binding affinity and their bioavailability via their compliance to Lipinski's rule of five. In this preliminary study, three candidates were selected based on their conforming to generated SERM's pharmacophore. They were further analyzed for their inhibition constant and their ability to select the binding mode of raloxifene over that of 4OH-tamoxifen. All candidates have shown inhibition constant in the micromolar and submicromolar range while one of the candidate shows selectivity to the prefer binding mode better than that of raloxifene. These results prove the validity of the generated pharmacophore. Further enhancement of current pharmacophore would result in more precise pharmacophore aiming for the next generation of SERMs ligands which have higher potency and tissue selectivity.

IT 835615-05-9
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(de Novo ligand design of selective estrogen receptor modulators)

RN 835615-05-9 CAPLUS

CN Formamide, N-[(2E,6E)-8-[2'-ethenyl-4',6'-dihydroxy-4-(nitrosomethyl)[1,1'-biphenyl]-2-yl]-5-ethyl-2,6,8-nonatrien-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 10 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:696360 CAPLUS Full-text

DOCUMENT NUMBER: 141:225492

TITLE: Preparation of isoxazoles as inhibitors of heat shock proteins

INVENTOR(S): Drysdale, Martin James; Dymock, Brian William; Finch, Harry; Webb, Paul; Mcdonald, Edward; James, Karen Elizabeth; Cheung, Kwai Ming; Mathews, Thomas Peter

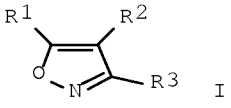
PATENT ASSIGNEE(S): Vernalis Cambridge Limited, UK; Cancer Research Technology Ltd; The Institute of Cancer Research; et al.; et al.

SOURCE: PCT Int. Appl., 180 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

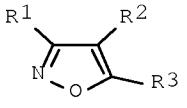
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004072051	A1	20040826	WO 2004-GB506	20040209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004210779	A1	20040826	AU 2004-210779	20040209
CA 2515726	A1	20040826	CA 2004-2515726	20040209
EP 1611112	A1	20060104	EP 2004-709273	20040209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1771235	A	20060510	CN 2004-80009339	20040209
JP 2006517572	T	20060727	JP 2006-502254	20040209
BR 2004007403	A	20061003	BR 2004-7403	20040209
MX 2005PA08335	A	20060504	MX 2005-PA8335	20050805
IN 2005CN01845	A	20070406	IN 2005-CN1845	20050808
NO 2005004195	A	20051109	NO 2005-4195	20050909
US 20060241106	A1	20061026	US 2006-544443	20060421

PRIORITY APPLN. INFO.:
GB 2003-3105 A 20030211
GB 2003-6560 A 20030321
GB 2003-13751 A 20030613
WO 2004-GB506 W 20040209

OTHER SOURCE(S): MARPAT 141:225492
GI



I

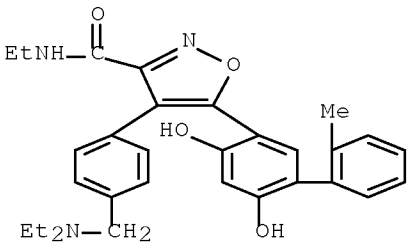


II

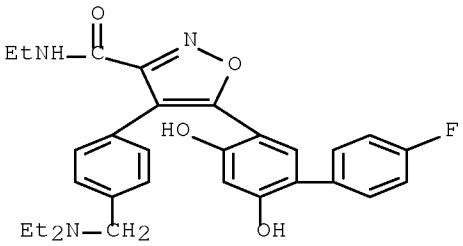
AB Title compds. [I, II; R1 = Ar1(Alk1)p(Z)r(Alk2)sQ; Ar1 = (substituted) aryl, heteroaryl; Alk1, Alk2 = (substituted) alkylene, alkenylene; p, r, s = 0, 1; Z = O, S, CO, CS, SO2, CO2, CONRA, CSNRA, SO2NRA, NRACO, NRASO2, NRA; RA = H, alkyl; Q = H, (substituted) carbocyclyl, heterocyclyl; R2 = Ar1(Alk1)p(Z)r(Alk2)sQ, carboxamide, carbocyclyl, heterocyclyl optionally substituted by (Alk1)pZr(Alk2)sQ; R3 = H, (substituted) cycloalkyl, cycloalkenyl, alkyl, alkenyl, alkynyl, carboxyl, carboxamide, carboxyl ester], were prepared Thus, NH2OH.HCl and 7-hydroxy-3-(4-methoxyphenyl)-2-methylchromen-4-one (preparation given) were refluxed 4 h in pyridine to give 4-[4-(4-methoxyphenyl)-3-methylisoxazol-5-yl]benzene-1,3-diol. The latter in the Malachite Green ATPase assay inhibited HSP90 with IC50 <50 μM.
IT 747412-67-5P 747412-68-6P 747412-69-7P

747412-70-0P 747412-71-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of isoxazoles as inhibitors of heat shock proteins)

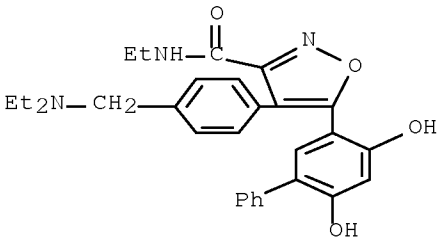
RN 747412-67-5 CAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-5-(4,6-dihydroxy-2'-methyl[1,1'-biphenyl]-3-yl)-N-ethyl- (CA INDEX NAME)



RN 747412-68-6 CAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)- (CA INDEX NAME)

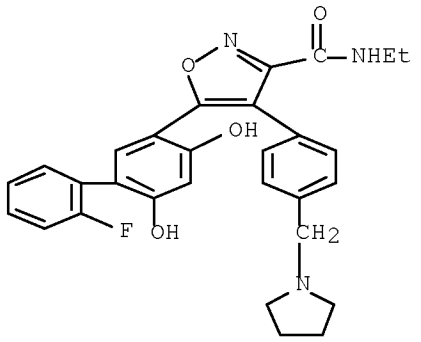


RN 747412-69-7 CAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl- (CA INDEX NAME)

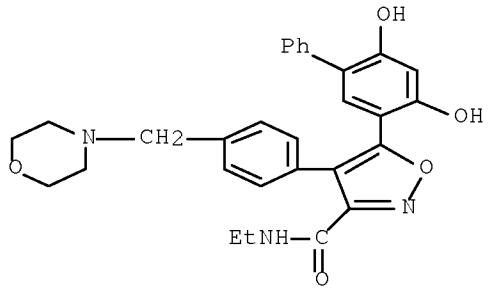


RN 747412-70-0 CAPLUS

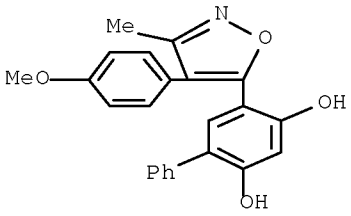
CN 3-Isoxazolecarboxamide, N-ethyl-5-(2'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(1-pyrrolidinylmethyl)phenyl]- (CA INDEX NAME)



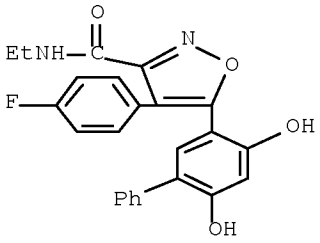
RN 747412-71-1 CAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-(4-morpholinylmethyl)phenyl]- (CA INDEX NAME)



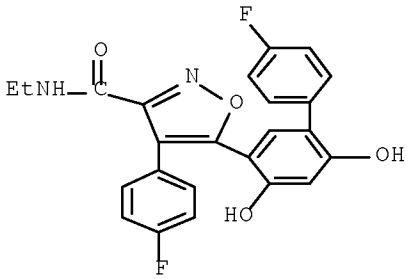
IT 747412-83-5P 747413-77-0P 747413-81-6P
747413-82-7P 747413-83-8P 747413-89-4P
747413-91-8P 747413-92-9P 747413-93-0P
747413-98-5P 747414-00-2P 747414-01-3P
747414-02-4P 747414-03-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoxazoles as inhibitors of heat shock proteins)
RN 747412-83-5 CAPLUS
CN [1,1'-Biphenyl]-2,4-diol, 5-[4-(4-methoxyphenyl)-3-methyl-5-isoxazolyl]- (CA INDEX NAME)



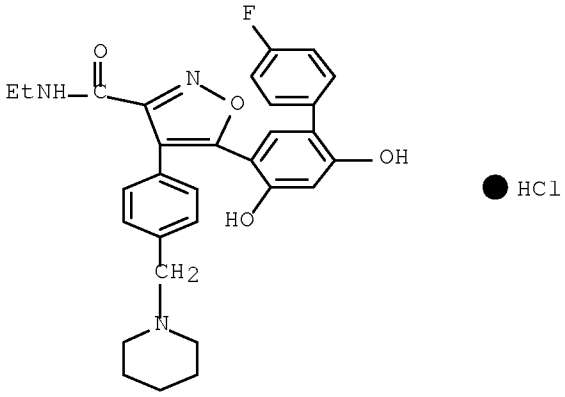
RN 747413-77-0 CAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-(4-fluorophenyl)- (CA INDEX NAME)



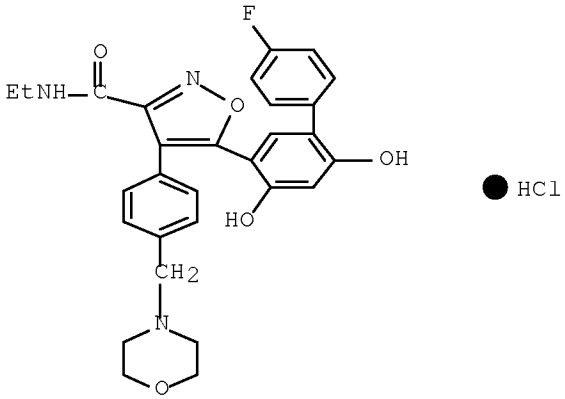
RN 747413-81-6 CAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-(4-fluorophenyl)- (CA INDEX NAME)



RN 747413-82-7 CAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(1-piperidinylmethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



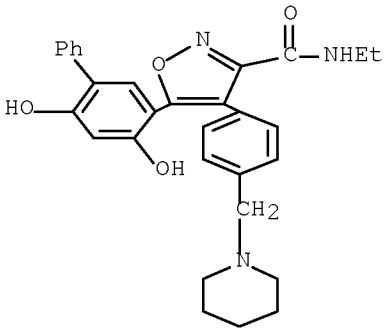
RN 747413-83-8 CAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(4-morpholinylmethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



RN 747413-89-4 CAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-(1-piperidinylmethyl)phenyl]-, acetate (1:1) (CA INDEX NAME)

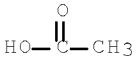
CM 1

CRN 747413-88-3
CMF C30 H31 N3 O4

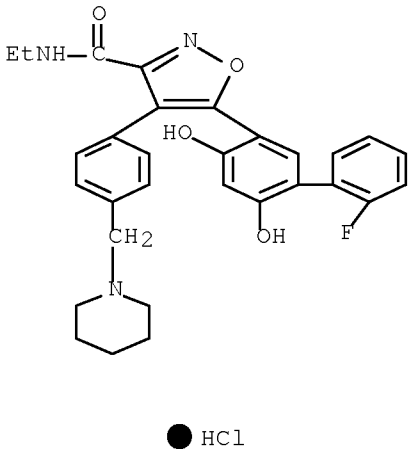


CM 2

CRN 64-19-7
CMF C2 H4 O2

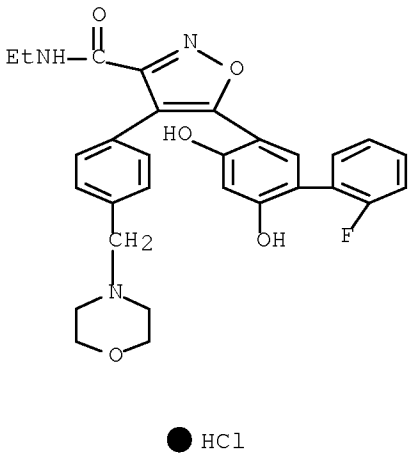


RN 747413-91-8 CAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(2'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(1-piperidinylmethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

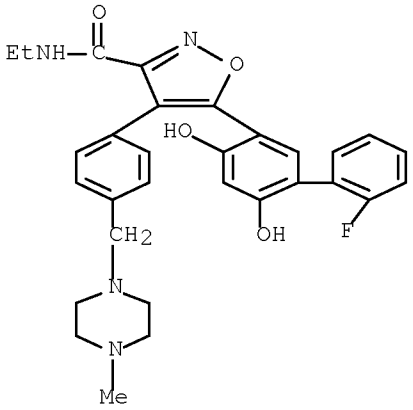


● HCl

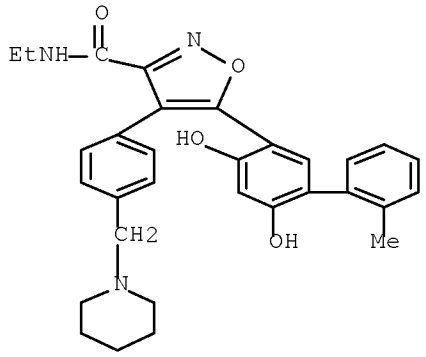
RN 747413-92-9 CAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(2'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(4-morpholinylmethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



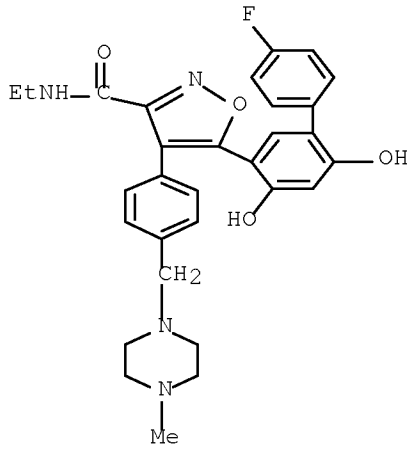
RN 747413-93-0 CAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(2'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]- (CA INDEX NAME)



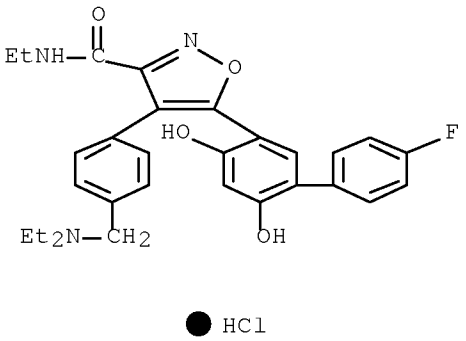
RN 747413-98-5 CAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy-2'-methyl[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-(1-piperidinylmethyl)phenyl]- (CA INDEX NAME)



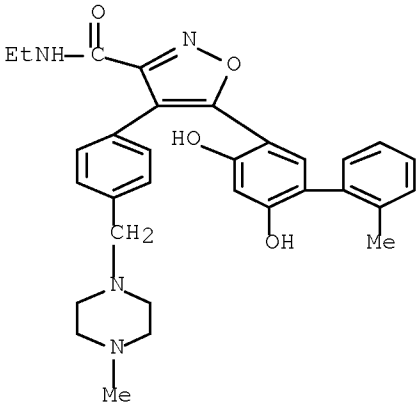
RN 747414-00-2 CAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]- (CA INDEX NAME)



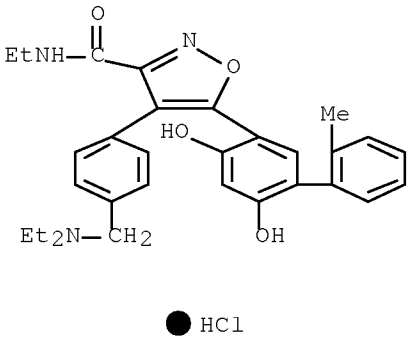
RN 747414-01-3 CAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-, hydrochloride (1:1) (CA INDEX NAME)



RN 747414-02-4 CAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy-2'-methyl[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]- (CA INDEX NAME)



RN 747414-03-5 CAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-5-(4,6-dihydroxy-2'-methyl[1,1'-biphenyl]-3-yl)-N-ethyl-, hydrochloride (1:1) (CA INDEX NAME)



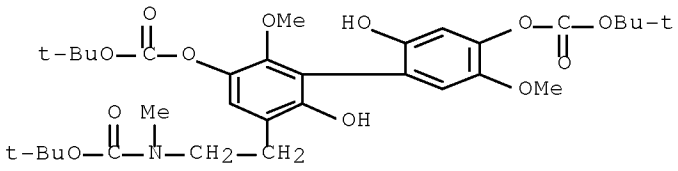
L19 ANSWER 11 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:555342 CAPLUS Full-text
DOCUMENT NUMBER: 139:323683
TITLE: Preparation of 6-phenyl- and 8-phenyl tetrahydro-isoquinolines from boldine
AUTHOR(S): Huang, Wei-Jan; Chen, Chung-Hsiung; Lee, Shoei-Sheng
CORPORATE SOURCE: School of Pharmacy, College of Medicine, National Taiwan University, Taipei, 100, Taiwan
SOURCE: Heterocycles (2003), 60(7), 1573-1588
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:323683
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four 6-phenyl- and 8-phenyltetrahydroisoquinolines, e.g. I (R = H, Me, Ph), were prepared by structural modifications of the boldine nucleus. These involved four major reaction steps, including solvolysis of the 2-hydroxyaporphine (boldine), ozonolysis of the C-9,10 double bond of the phenanthrene nucleus in secoboldine derivative II, leading to the key intermediate, dialdehyde III, and final Pictet-Spengler cyclization to resp. target products.

IT 613223-27-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenylisoquinolines from boldine via solvolysis of hydroxyaporphine, ozonolysis, and Pictet-Spengler cyclization)

RN 613223-27-1 CAPLUS
CN Carbonic acid, 5-[2-[[(1,1-dimethylethoxy)carbonyl]methylamino]ethyl]-2',6-dihydroxy-2,5'-dimethoxy[1,1'-biphenyl]-3,4'-diyl bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 12 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:532647 CAPLUS Full-text
DOCUMENT NUMBER: 139:101122
TITLE: Preparation of 3,4-diarylpyrazoles as inhibitors of heat shock protein 90 (HSP90) and their use in the therapy of cancer

INVENTOR(S): Drysdale, Martin James; Dymock, Brian William; Barril-Alonso, Xavier; Workman, Paul; Pearl, Laurence Harris; Prodromou, Chrisostomos; MacDonald, Edward

PATENT ASSIGNEE(S): Ribotargets Limited, UK; Cancer Research Technology Limited; The Institute of Cancer Research

SOURCE: PCT Int. Appl., 299 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

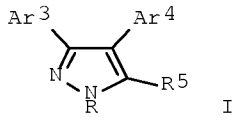
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003055860	A1	20030710	WO 2002-GB5778	20021219
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002356301	A1	20030715	AU 2002-356301	20021219
EP 1456180	A1	20040915	EP 2002-805823	20021219
EP 1456180	B1	20071003		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005517675	T	20050616	JP 2003-556391	20021219
AT 374753	T	20071015	AT 2002-805823	20021219
US 20050222230	A1	20051006	US 2005-499030	20050425
US 7247734	B2	20070724		

PRIORITY APPLN. INFO.:	GB 2001-30733	A	20011221
	GB 2002-25688	A	20021104
	WO 2002-GB5778	W	20021219

OTHER SOURCE(S): MARPAT 139:101122

GI



I

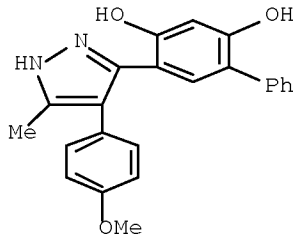
AB A method of inhibiting HSP90 comprises administration of title compds. [I; Ar3, Ar4 = (substituted) C5-20 aryl; R5 = H, halo, OH, ether, formyl, acyl, CO2H, ester, acyloxy, oxycarbonyloxy, amido, acylamido, aminocarbonyloxy, tetrazolyl, amino, NO2, cyano, N3, sulfhydryl, thioether, sulfonamido, C1-7 alkyl, C3-20 heterocyclyl, C5-20 aryl; R = H, C1-7 alkyl, C3-20 heterocyclyl, C5-20 aryl] and pharmaceutically acceptable salts, solvates, amides, esters, ethers, chemical protected forms, and prodrugs thereof. Thus, 7-hydroxy-3-phenylchromen-4-one and hydrazine hydrate were refluxed 45 min. in EtOH to

give 4-(4-phenyl-1H-pyrazol-3- yl)benzene-1,3-diol. This inhibited HSP90 activity with IC50 = 10-100 μM.

IT 558638-25-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diarylpyrazoles as inhibitors of heat shock protein 90 and their use in the therapy of cancer)

RN 558638-25-8 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-[4-(4-methoxyphenyl)-5-methyl-1H-pyrazol-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 13 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:472498 CAPLUS Full-text

DOCUMENT NUMBER: 139:36523

TITLE: Preparation of thiazolidinones and oxazolidinones for the inhibition of phosphatases and the treatment of cancer

INVENTOR(S): Pfahl, Magnus; Al-shamma, Hussien A.; Fanjul, Andrea N.; Pleynet, David P. M.; Bao, Haifeng; Spruce, Lyle W.; Cow, Christopher N.; Tachdjian, Catherine; Zapt, James W.; Wiemann, Torsten R.

PATENT ASSIGNEE(S): Maxia Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 182 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003050098	A1	20030619	WO 2002-US39178	20021206

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2469342	A1	20030619	CA 2002-2469342	20021206
AU 2002357098	A1	20030623	AU 2002-357098	20021206
US 20040097566	A1	20040520	US 2002-313341	20021206
EP 1463718	A1	20041006	EP 2002-804747	20021206

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

PRIORITY APPLN. INFO.: US 2001-337195P P 20011206
WO 2002-US39178 W 20021206

OTHER SOURCE(S): MARPAT 139:36523

GI

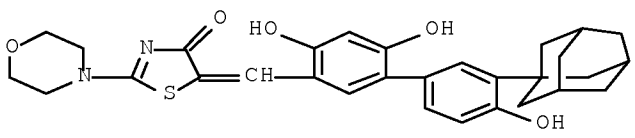
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title heterocycles I and II [wherein Ar1 = (un)substituted Ph; Ar2 = (un)substituted (hetero)aryl; R1 = H, OH, alkoxy, or (un)substituted alkyl; W = S or O; X = S or O; Y = organic radical comprising 1-15 C atoms; and pharmaceutically acceptable salts thereof] were prepared as phosphatase inhibitors. For example, 3-fluoro-4-hydroxybromobenzene was alkylated with 1-adamantanol to give 3-(adamantan-1-yl)-4-hydroxy-5- fluorobromobenzene (45%), which was O-protected with t-butyldimethylsilyl chloride (94%). Coupling with 3-formylphenylboronic acid in the presence of Na2CO3 and Pd(PPh3)4 in toluene, EtOH, and H2O afforded the substituted benzaldehyde (77%). Deprotection (80%) followed by condensation with rhodanine and reaction with morpholine in AcOH and toluene provided III (73%). Representative compds. of the invention inhibited recombinant human Cdc25A at concns. of 1 μM and 10 μM and killed significant percentages of breast cancer, prostate cancer, non-small-cell lung cancer, and pancreatic cancer cells at concns. in the range of 10-7 M to 10-5 M or higher. Thus, I, II, and pharmaceutical compns. thereof are useful in the treatment of diseases related to uncontrolled cellular proliferation, such as cancer or precancerous conditions. In addition, I and II are also useful for modulating lipid and/or carbohydrate metabolism, and treating Type II diabetes, hyperglycemia, or obesity, and for treating inflammatory diseases, such as arthritis (no data).

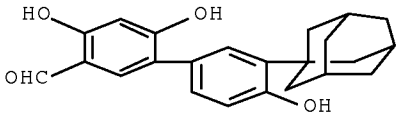
IT 544475-00-5P, 5-[3-[3-(Adamantan-1-yl)-4-hydroxyphenyl]-4,6-dihydroxybenzylidene]-2-(morpholin-4-yl)thiazol-4-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phosphatase inhibitor; preparation of thiazolidinone and oxazolidinone phosphatase inhibitors for treatment of cancer, diabetes, and inflammatory diseases)

RN 544475-00-5 CAPLUS

CN 4(5H)-Thiazolone, 2-(4-morpholinyl)-5-[(4,4',6-trihydroxy-3'-tricyclo[3.3.1.13,7]dec-1-yl[1,1'-biphenyl]-3-yl)methylene]- (CA INDEX NAME)

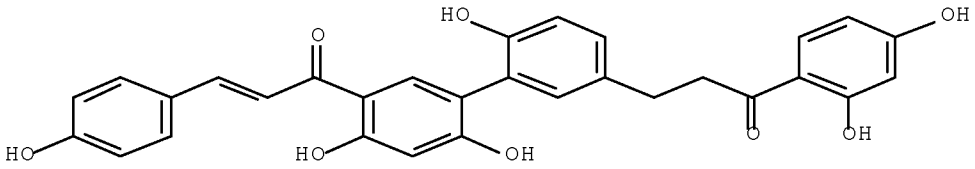


IT 544475-01-6, 3-[3-(Adamantan-1-yl)-4-hydroxyphenyl]-4,6-dihydroxybenzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiazolidinone and oxazolidinone phosphatase inhibitors for treatment of cancer, diabetes, and inflammatory diseases)
RN 544475-01-6 CAPLUS
CN [1,1'-Biphenyl]-3-carboxaldehyde, 4,4',6-trihydroxy-3'-tricyclo[3.3.1.13,7]dec-1-yl- (CA INDEX NAME)

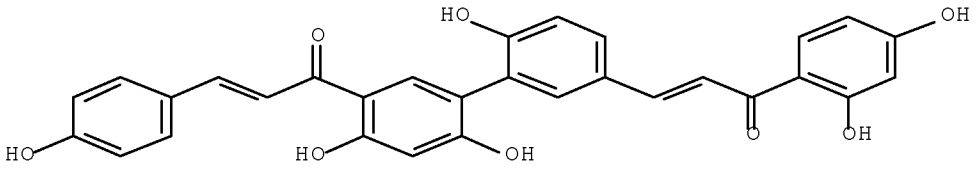


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 14 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:295435 CAPLUS Full-text
DOCUMENT NUMBER: 139:33303
TITLE: Rhuschalcones II-VI, Five New Bichalcones from the Root Bark of Rhus pyroides
AUTHOR(S): Mdee, Ladislaus K.; Yeboah, Samuel O.; Abegaz, Berhanu M.
CORPORATE SOURCE: Department of Chemistry, University of Botswana, Gaborone, Botswana
SOURCE: Journal of Natural Products (2003), 66(5), 599-604
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Biflavonoids detected in trace amts. in an earlier investigation of the twigs of Rhus pyroides have now been found in the root bark of this species. These new flavonoids belong to a rare bichalcone class and have been identified as 2',4',4'',2''',4'''-pentahydroxy-4-O-5'''-bichalcone (rhuschalcone II, 2), 2',4',4'',2'''-tetrahydroxy-4'''-methoxy-4-O-5'''- bichalcone (rhuschalcone III, 3), 4,2',4'',2'''-tetrahydroxy-4'''-methoxy- 4'-O-5'''-bichalcone (rhuschalcone IV, 4), 4,2',4',4'',2''',4'''- hexahydroxy-3,5'''-dihydrochalcone-chalcone (rhuschalcone V, 5), and 4,2',4',4'',2''',4'''-hexahydroxy-3,5'''-bichalcone (rhuschalcone VI, 6), resp. Also obtained was the known compound rhuschalcone I (1). Their structures were determined by spectroscopic and chemical methods, and for 1-3 by total synthesis. All the bichalcones (1-6) tested exhibited selective cytotoxic activity against the HT29 and HCT-116 colon tumor cell lines.
IT 541502-83-4P, Rhuschalcone V 541502-84-5P, Rhuschalcone VI
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(new bichalcones rhuschalcones II-VI from root bark of Rhus pyroides)
RN 541502-83-4 CAPLUS
CN 2-Propen-1-one, 1-[5'-[3-(2,4-dihydroxyphenyl)-3-oxopropyl]-2',4,6-trihydroxy[1,1'-biphenyl]-3-yl]-3-(4-hydroxyphenyl)-, stereoisomer (9CI) (CA INDEX NAME)



RN 541502-84-5 CAPLUS
CN 2-Propen-1-one, 1-[5'-[(1E)-3-(2,4-dihydroxyphenyl)-3-oxo-1-propen-1-yl]-2',4,6-trihydroxy[1,1'-biphenyl]-3-yl]-3-(4-hydroxyphenyl)-, (2E)-(-)- (CA INDEX NAME)

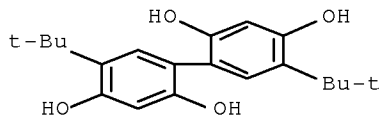


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 15 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:53748 CAPLUS Full-text
DOCUMENT NUMBER: 138:237722
TITLE: Copper(II)-Mediated Autoxidation of tert-Butylresorcinols
AUTHOR(S): Ling, Ke-Qing; Lee, Younghee; Macikenas, Dainius; Protasiewicz, John D.; Sayre, Lawrence M.
CORPORATE SOURCE: Department of Chemistry, Case Western Reserve University, Cleveland, OH, 44106, USA
SOURCE: Journal of Organic Chemistry (2003), 68(4), 1358-1366
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:237722

AB Although copper(II)-mediated oxidation of phenols results in oxidative coupling rather than in oxygenation, it was recently reported that naturally occurring 5-alkylresorcinols undergo oxygenation in the presence of copper(II). To explore the generality of this reaction, the copper(II)-mediated autoxidn. of 4-tert-butylresorcinol and 4,6-di-tert-butylresorcinol was investigated and was found to result in direct oxygenation at open activated positions and, at the tert-butyl-substituted positions, in oxygenation with competing loss of (as isobutylene) and 1,2-rearrangement of the tert-Bu group. 5-tert-Butyl-2-hydroxy-1,4-benzoquinone is the major product from both starting materials, and the final product mixture reflects, in part, coupling of metastable initially formed electrophilic and nucleophilic side products. Mechanisms that are consistent with the observed products and control reactions are proposed. The key step appears to be equilibration of a copper(II)-resorcinolate with a charge-transfer radical form that reacts regioselectively with O2 as prescribed by resonance.

IT 501668-41-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(autoxidn. of butylresorcinol derivs. by Cu mediation)
RN 501668-41-3 CAPLUS
CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 5,5'-bis(1,1-dimethylethyl)- (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 16 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:927396 CAPLUS Full-text
DOCUMENT NUMBER: 138:13955
TITLE: Preparation of phenol and hydroxynaphthalene based inhibitors of protein kinase for the treatment of disease
INVENTOR(S): Cao, Sheldon Xiaodong; Bounaud, Pierre-Yves; Chen, Xiaohua; Chung, Hyun-Ho; Dumas, David Paul; Kc, Sunil Kumar; Min, Changhee; Yang, Jae Young; Long, Mellissa C.
PATENT ASSIGNEE(S): LG Biomedical Institute, USA
SOURCE: PCT Int. Appl., 286 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002096867	A2	20021205	WO 2002-US16920	20020528
WO 2002096867	A3	20040304		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002310187	A1	20021209	AU 2002-310187	20020528
US 20030187007	A1	20031002	US 2002-158030	20020528
US 20030208067	A1	20031106	US 2002-158103	20020528
EP 1412327	A2	20040428	EP 2002-737248	20020528
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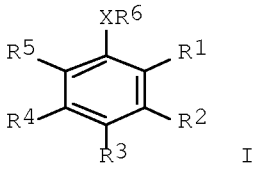
JP 2004534779	T	20041118	JP 2003-500047	20020528
KR 2004026657	A	20040331	KR 2003-715388	20031125
PRIORITY APPLN. INFO.:			US 2001-294792P P	20010530

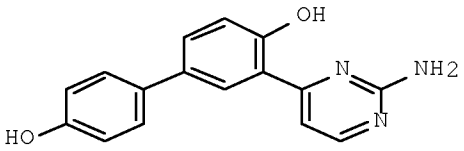
WO 2002-US16920 W 20020528

OTHER SOURCE(S): MARPAT 138:13955

GI



I



II

AB Phenol and hydroxynaphthalene derivs. I [X = O, S, amine, alkylamine, alkynylamine, arylamine, and heteroarylamine; R1 = (un)substituted 5- or 6-membered aromatic or heteroarom. ring, -(X1)mCOX2-, wherein X1 = alkylene, alkenylene, alkynylene, aryl and heteroaryl, X2 = H, alkyl, aryl, heteroaryl, OH, alkoxy, amino, substituted amine, m = 0 or 1, or R1 = -C(X3)=N-NX4-C(=E)-NX5X6 wherein X3 = H, alkyl, aryl, alkylaryl, heteroaryl, and amino and E = O, S, and substituted amine with X4, X5, and X6 independently equal to H, alkyl, aryl, and heteroaryl; R2, R3, and R4 = H, alkyl, alkylene, halo, alkoxy, etc.; or R2 and R3 or R3 and R4 may be taken together to form an (un)substituted aromatic or heteroarom. ring; R5 = H, (un)substituted-alkyl, -aryl, -heterocycle, etc.; R6 = H, alkyl, alkene, alkyne, aryl, and heteroaryl] are prepared and disclosed as inhibitors of protein kinase. Thus, II was prepared by cyclocondensation of 5'-bromo-2'-methoxyacetophenone with N,N-dimethylformamide di-Et acetal with subsequent Suzuki coupling with 4-methoxyphenylboronic acid. In assays to determine cyclin dependent kinase activity, specifically against CDK2 and CDK5, II possessed IC50 values of 0-0.5 μM. II proved highly specific for CDK2 and CDK5 and was further evaluated by in vitro tumor cell efficacy tests against numerous cancers. The present invention is directed in part towards methods of modulating the function of protein kinases with phenol- and hydroxynaphthalene-based compds. The methods incorporate cells that express a protein kinase. In addition, the invention describes methods of preventing and treating protein kinase-related abnormal conditions in organisms with a compound identified by the invention. Furthermore, the invention pertains to phenol- and hydroxynaphthalene-based compds. and pharmaceutical compns. comprising these compds.

IT 477726-38-8P 477726-39-9P

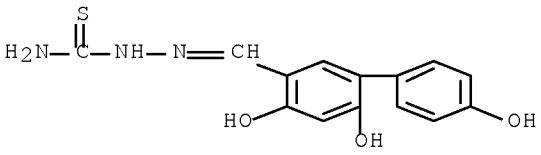
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of phenol and hydroxynaphthalene based inhibitors of protein kinase)

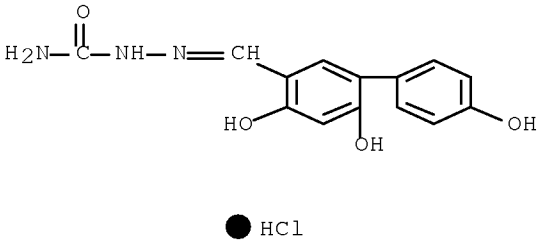
RN 477726-38-8 CAPLUS

CN Hydrazinecarbothioamide, 2-[(4,4',6-trihydroxy[1,1'-biphenyl]-3-

yl)methylene]- (CA INDEX NAME)



RN 477726-39-9 CAPLUS
CN Hydrazinecarboxamide, 2-[(4,4',6-trihydroxy[1,1'-biphenyl]-3-yl)methylene]-, hydrochloride (1:1) (CA INDEX NAME)



L19 ANSWER 17 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:868162 CAPLUS Full-text
DOCUMENT NUMBER: 136:5987
TITLE: Thrombopoietin mimetics
INVENTOR(S): Duffy, Kevin J.; Erickson-Miller, Connie L.; Eppley, Daniel F.; Jenkins, Julian; Luengo, Juan I.; Liu, Nannan; Price, Alan T.; Shaw, Antony N.; Visonneau, Sophie; Wiggall, Kenneth
PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA; Glaxo Group Limited
SOURCE: PCT Int. Appl., 114 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001089457	A2	20011129	WO 2001-US16863	20010524
WO 2001089457	A3	20020307		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,

BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2411468	A1	20011129	CA 2001-2411468	20010524
CA 2411468	C	20080415		
AU 2001074938	A	20011203	AU 2001-74938	20010524
EP 1294378	A2	20030326	EP 2001-941599	20010524
EP 1294378	B1	20071003		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001011116	A	20030408	BR 2001-11116	20010524
HU 2003002257	A2	20031028	HU 2003-2257	20010524
HU 2003002257	A3	20070328		
JP 2003534257	T	20031118	JP 2001-585703	20010524
JP 3813875	B2	20060823		
NZ 522474	A	20041029	NZ 2001-522474	20010524
NZ 533308	A	20051028	NZ 2001-533308	20010524
AU 2001274938	B2	20060119	AU 2001-274938	20010524
AT 374772	T	20071015	AT 2001-941599	20010524
EP 1864981	A1	20071212	EP 2007-112105	20010524
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EP 1889838	A1	20080220	EP 2007-112106	20010524
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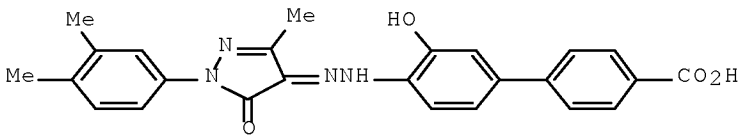
ES 2294000	T3	20080401	ES 2001-941599	20010524
NO 2002005566	A	20030122	NO 2002-5566	20021120
NO 324246	B1	20070917		
IN 2002MN01666	A	20041211	IN 2002-MN1666	20021121
KR 798568	B1	20080128	KR 2002-715869	20021123
ZA 2002009561	A	20031020	ZA 2002-9561	20021125
MX 2002PA11621	A	20040517	MX 2002-PA11621	20021125
US 20040019190	A1	20040129	US 2003-296688	20030703
US 7160870	B2	20070109		
HK 1055561	A1	20080411	HK 2003-106428	20030909
JP 2006137764	A	20060601	JP 2005-353686	20051207
US 20070179192	A1	20070802	US 2006-558071	20061109
US 7335649	B2	20080226		
US 20070129338	A1	20070607	US 2007-620260	20070105
US 7332481	B2	20080219		
US 20080090996	A1	20080417	US 2007-650688	20070108
US 20080090787	A1	20080417	US 2007-650838	20070108
US 20080214640	A1	20080904	US 2007-650651	20070108
KR 2007087255	A	20070827	KR 2007-718036	20070806
KR 847172	B1	20080717		

PRIORITY APPLN. INFO.:

US 2000-207084P	P	20000525
US 2000-228929P	P	20000830
EP 2001-941599	A3	20010524
JP 2001-585703	A3	20010524
WO 2001-US16863	W	20010524
KR 2002-715869	A3	20021123
US 2003-296688	A1	20030703

OTHER SOURCE(S): MARPAT 136:5987

GI



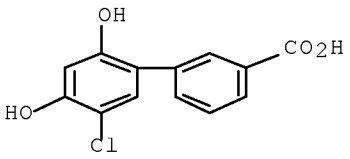
I

AB Pyrazolylidenehydrazino compds. such as I were prepared as thrombopoietin mimetics. Thus, I was prepared in 5 steps, the last of which involved reaction of 4-amino-3'-hydroxy-3-biphenylcarboxylic acid hydrochloride with 1-(3,4-dimethylphenyl)-3-methyl-3-pyrazolin-5-one.

IT 376594-19-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
((pyrazolylidenehydrazino)phenol derivs. as thrombopoietin mimetics)

RN 376594-19-3 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 5'-chloro-2',4'-dihydroxy- (CA INDEX NAME)



L19 ANSWER 18 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:359840 CAPLUS Full-text

DOCUMENT NUMBER: 134:366682

TITLE: Oncolytic combinations for the treatment of cancer

INVENTOR(S): Sawyer, Jason Scott; Teicher, Beverly Ann; Beight, Douglas Wade; Smith, Edward C. R.; McMillen, William Thomas

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 270 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001034198	A2	20010517	WO 2000-US30941	20001109
WO 2001034198	A3	20020214		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-164900P P 19991111

OTHER SOURCE(S): MARPAT 134:366682

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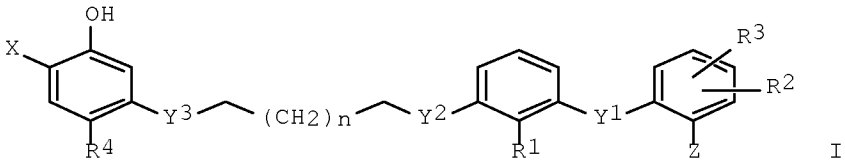

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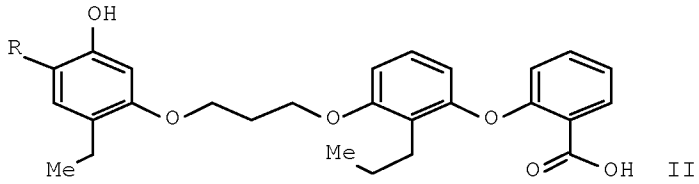


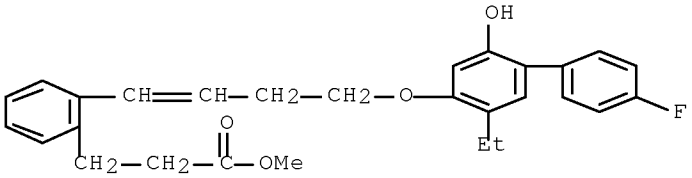
II

AB A method of treating cancer that comprises administering a patient ionizing radiation in conjunction with effective amts. of a 2',2'-difluoronucleoside anti-cancer compound and a leukotriene LTB4 inhibitor (I) [wherein X = a 5-membered (un)substituted heterocycle or fused bicyclic radical consisting of a carbocyclic group fused to 2 adjacent C atoms of a 5-membered (un)substituted heterocycle; Y1 = a bond or divalent linking group containing 1-9 atoms; Y2 and Y3 = independently CH2, O, or S; Z = an acidic group; R1 = (alk)aryl, cycloalkyl, (ar)alkyl, (ar)alkenyl, alkynyl, haloalkyl, aryloxy, or alkoxy; R2 = H, halo(alkyl), alkoxy, (cyclo)alkyl, acidic group, or (CH2)1-7-acidic group; R3 = (cyclo)alkyl, (CH2)1-7-cycloalkyl, alkenyl, alkynyl, benzyl, or aryl; n = 0-6] is disclosed. Examples includes 17 syntheses, 22 formulations, and Lewis lung test results. For instance, benzylation of 1-[2-hydroxy-4-(3-chloropropoxy)-5-ethylphenyl]ethanone (69%), coupling the ethanone with 2-(3-hydroxy-2-propylphenoxy)benzoic acid Me ester (72%), oxidation to give the α-hydroxy ketone (31%), cyclization with triflic anhydride and formamide to give the oxazole (6%), debenzylation with BF3•OEt2 (45%), and deesterification (92%) afforded II (R = 4-oxazolyl). Treatment of C57B1 mice with 100 mg/kg of the LTB4 antagonist, 2-[2-propyl-3-[3-[2-ethyl-5-hydroxy-4-(4-fluorophenyl)phenoxy]propoxy]phenoxy]benzoic acid (II; R = 4-FC6H4), 60 mg/kg of gemcitabine•HCl, and 400 Rads of radiation delayed growth of murine Lewis lung carcinoma by an average of 32.3 days, compared to a delay of 13.4 days using the gemcitabine•HCl and radiation combination. In addition, the mean number of lung metastases was reduced from 11.5 to 7.0.

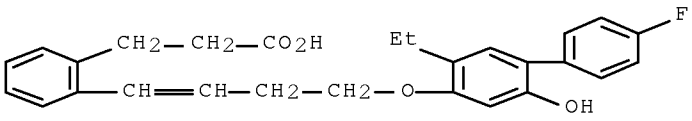
IT 152607-86-8, Methyl 3-[2-[4-[2-ethyl-4-(4-fluorophenyl)-5-hydroxyphenoxy]-1-butenyl]phenyl]propionate 185394-53-0, 3-[2-[4-[2-Ethyl-4-(4-fluorophenyl)-5-hydroxyphenoxy]-1-butenyl]phenyl]propionic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of phenoxyalkoxyphenoxybenzoic acids and analogs as leukotriene antagonists for use with 2',2'-difluoronucleoside anti-cancer agents and radiation therapy for treatment of cancer)

RN 152607-86-8 CAPLUS

CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]-, methyl ester (CA INDEX NAME)



RN 185394-53-0 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]- (CA INDEX NAME)

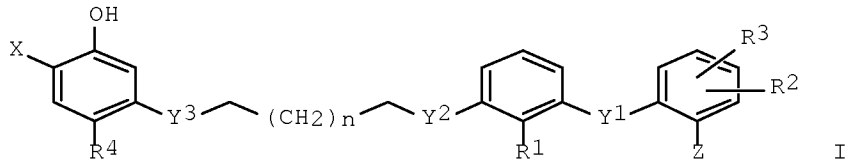


L19 ANSWER 19 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:359839 CAPLUS Full-text
DOCUMENT NUMBER: 134:366681
TITLE: Oncolytic combinations for the treatment of cancer
INVENTOR(S): Sawyer, Jason Scott; Teicher, Beverly Ann; Beight, Douglas Wade; Smith, Edward C. R.; McMillen, William Thomas
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 250 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001034197	A2	20010517	WO 2000-US30839	20001109
WO 2001034197	A3	20020510		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-164704P P 19991111
OTHER SOURCE(S): MARPAT 134:366681
GI



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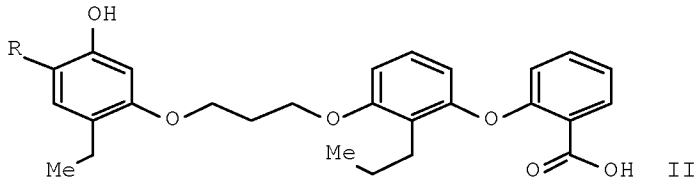


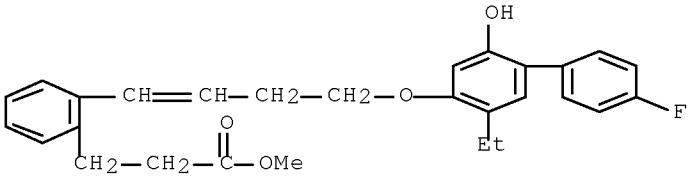
II

AB A method of treating cancer with radiation in conjunction with the administration of a leukotriene LTB4 inhibitor (I) [wherein X = a 5-membered (un)substituted heterocycle or fused bicyclic radical consisting of a carbocyclic group fused to 2 adjacent C atoms of a 5-membered (un)substituted heterocycle; Y1 = a bond or divalent linking group containing 1-9 atoms; Y2 and Y3 = independently CH2, O, or S; Z = an acidic group; R1 = (alk)aryl, cycloalkyl, (ar)alkyl, (ar)alkenyl, alkynyl, haloalkyl, aryloxy, or alkoxy; R2 = H, halo(alkyl), alkoxy, (cyclo)alkyl, acidic group, or (CH2)1-7-acidic group; R3 = (cyclo)alkyl, (CH2)1-7-cycloalkyl, alkenyl, alkynyl, benzyl, or aryl; n = 0-6] is disclosed. Examples includes 17 syntheses, 7 formulations, nude mouse xenograft test results, and Lewis lung test results. For instance, benzylation of 1-[2-hydroxy-4-(3-chloropropoxy)-5-ethylphenyl]ethanone (69%), coupling the ethanone with 2-(3-hydroxy-2-propylphenoxy)benzoic acid Me ester (72%), oxidation to give the α-hydroxy ketone (31%), cyclization with triflic anhydride and formamide to give the oxazole (6%), debenzylation with BF3•OEt2 (45%), and deesterification (92%) afforded II (R = 4-oxazolyl). Treatment of mice with 100 mg/kg of the LTB4 antagonist, 2-[2-propyl-3-[3-[2-ethyl-5-hydroxy-4-(4- fluorophenyl)phenoxy]propoxy]phenoxy]benzoic acid (II; R = 4-FC6H4) and 400 Rads of radiation delayed growth of human DU145 prostate carcinoma by an average of 31.5 days, compared to a delay of 19.2 days using radiation alone. In the Lewis lung test, the mean number of lung metastases was reduced from 15.5 using radiation alone to 12.0 using the combination therapy.

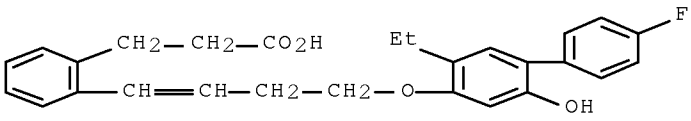
IT 152607-86-8, Methyl 3-[2-[4-[2-ethyl-4-(4-fluorophenyl)-5-hydroxyphenoxy]-1-butenyl]phenyl]propionate 185394-53-0, 3-[2-[4-[2-Ethyl-4-(4-fluorophenyl)-5-hydroxyphenoxy]-1-butenyl]phenyl]propionic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation and use of phenoxyalkoxyphenoxybenzoic acids and analogs as leukotriene antagonists in conjunction with radiation therapy for treatment of cancer)

RN 152607-86-8 CAPLUS

CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]-, methyl ester (CA INDEX NAME)



RN 185394-53-0 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]- (CA INDEX NAME)



L19 ANSWER 20 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:359787 CAPLUS Full-text
DOCUMENT NUMBER: 134:366680
TITLE: Oncolytic combinations for the treatment of cancer
INVENTOR(S): Fleisch, Jerome Herbert; Benjamin, Roger Stuart; Sawyer, Jason Scott; Teicher, Beverly Ann; Beight, Douglas Wade; Smith, Edward C. R.; McMillen, William Thomas
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 283 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001034137	A2	20010517	WO 2000-US31039	20001109
WO 2001034137	A3	20020214		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2391416	A1	20010517	CA 2000-2391416	20001109
AU 2001015990	A	20010606	AU 2001-15990	20001109
AU 778829	B2	20041223		
BR 2000015490	A	20020709	BR 2000-15490	20001109
EP 1231938	A2	20020821	EP 2000-978535	20001109
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2003513916	T	20030415	JP 2001-536137		20001109
HU 2002004449	A2	20030428	HU 2002-4449		20001109
HU 2002004449	A3	20060228			
NZ 517667	A	20040528	NZ 2000-517667		20001109
TR 200201245	T2	20040823	TR 2002-1245		20001109
ZA 2002002822	A	20030710	ZA 2002-2822		20020410
NO 2002002245	A	20020709	NO 2002-2245		20020510
MX 2002PA04733	A	20020830	MX 2002-PA4733		20020510
PRIORITY APPLN. INFO.:			US 1999-164786P	P	19991111
			WO 2000-US31039	W	20001109

OTHER SOURCE(S): MARPAT 134:366680

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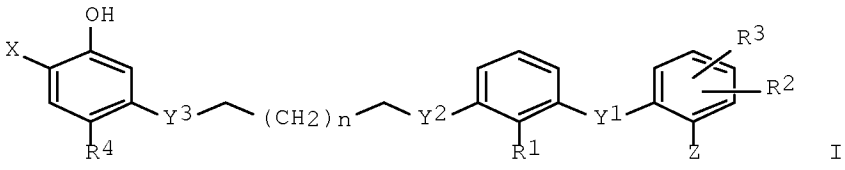

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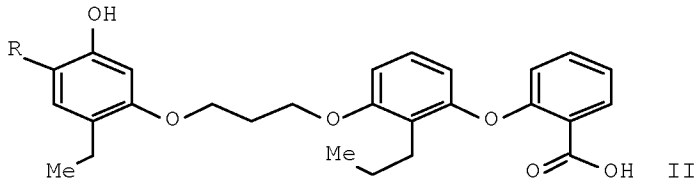


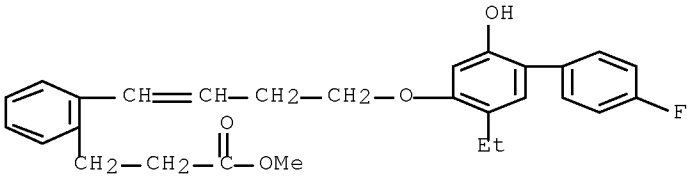
II

AB A method of treating cancer by administration of a 2',2'- difluoronucleoside anti-cancer compound and a leukotriene LTB4 inhibitor (I) [wherein X = a 5-membered (un)substituted heterocycle or fused bicyclic radical consisting of a carbocyclic group fused to 2 adjacent C atoms of a 5-membered (un)substituted heterocycle; Y1 = a bond or divalent linking group containing 1-9 atoms; Y2 and Y3 = independently CH2, O, or S; Z = an acidic group; R1 = (alk)aryl, cycloalkyl, (ar)alkyl, (ar)alkenyl, alkynyl, haloalkyl, aryloxy, or alkoxy; R2 = H, halo(alkyl), alkoxy, (cyclo)alkyl, acidic group, or (CH2)1-7-acidic group; R3 = (cyclo)alkyl, (CH2)1-7-cycloalkyl, alkenyl, alkynyl, benzyl, or aryl; n = 0-6] is disclosed. Examples includes 17 syntheses, 22 formulations, and mouse xenograft test results. For instance, benzylation of 1-[2-hydroxy-4-(3- chloropropoxy)-5-ethylphenyl]ethanone (69%), coupling the ethanone with 2-(3-hydroxy-2-propylphenoxy)benzoic acid Me ester (72%), oxidation to give the α-hydroxy ketone (31%), cyclization with triflic anhydride and formamide to give the oxazole (6%), debenzylation with BF3•OEt2 (45%), and deesterification (92%) afforded II (R = 4-oxazolyl). Treatment of mice with 100 mg/kg of the LTB4 antagonist, 2-[2-propyl-3-[3-[2-ethyl-5- hydroxy-4-(4-fluorophenyl)phenoxy]propoxy]phenoxy]benzoic acid (II; R = 4-FC6H4) and 60 mg/kg of gemcitabine•HCl delayed growth of LNCaP prostate carcinoma by an average of 51.2 days, compared to a delay of 12.2 days using the gemcitabine•HCl alone.

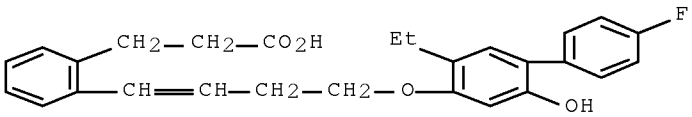
IT 152607-86-8, Methyl 3-[2-[4-[2-ethyl-4-(4-fluorophenyl)-5-hydroxyphenoxy]-1-butenyl]phenyl]propionate 185394-53-0, 3-[2-[4-[2-Ethyl-4-(4-fluorophenyl)-5-hydroxyphenoxy]-1-

butenyl]phenyl]propionic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of phenoxyalkoxyphenoxybenzoic acids and analogs as leukotriene antagonists for use with 2',2'-difluoronucleoside anti-cancer agents for treatment of cancer)

RN 152607-86-8 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]-, methyl ester (CA INDEX NAME)



RN 185394-53-0 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]- (CA INDEX NAME)



L19 ANSWER 21 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:359785 CAPLUS Full-text
DOCUMENT NUMBER: 134:366679
TITLE: Oncolytic combinations for the treatment of cancer
INVENTOR(S): Fleisch, Jerome Herbert; Sawyer, Jason Scott; Teicher, Beverly Ann; Beight, Douglas Wade; Smith, Edward C. R.; McMillen, William Thomas
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 285 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001034135	A2	20010517	WO 2000-US30944	20001109
WO 2001034135	A3	20020321		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,

SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2390789	A1	20010517	CA 2000-2390789		20001109
EP 1231939	A2	20020821	EP 2000-983695		20001109
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2003513914	T	20030415	JP 2001-536135		20001109
PRIORITY APPLN. INFO.:			US 1999-164713P	P	19991111
			WO 2000-US30944	W	20001109

OTHER SOURCE(S): MARPAT 134:366679
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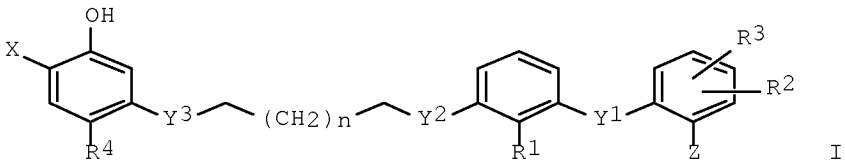

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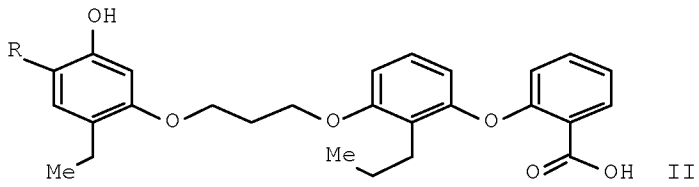


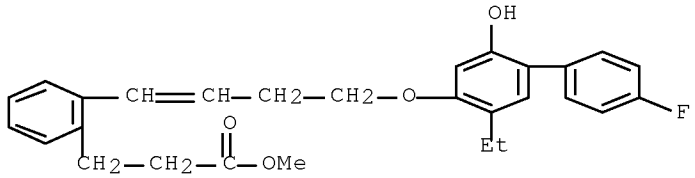
II

AB A method of treating cancer with therapeutic combinations of a leukotriene LTB4 inhibitor (I) [wherein X = a 5-membered (un)substituted heterocycle or fused bicyclic radical consisting of a carbocyclic group fused to 2 adjacent C atoms of a 5-membered (un)substituted heterocycle; Y1 = a bond or divalent linking group containing 1-9 atoms; Y2 and Y3 = independently CH2, O, or S; Z = an acidic group; R1 = (alk)aryl, cycloalkyl, (ar)alkyl, (ar)alkenyl, alkynyl, haloalkyl, aryloxy, or alkoxy; R2 = H, halo(alkyl), alkoxy, (cyclo)alkyl, acidic group, or (CH2)1-7-acidic group; R3 = (cyclo)alkyl, (CH2)1-7-cycloalkyl, alkenyl, alkynyl, benzyl, or aryl; n = 0-6] and an anti-cancer agent is disclosed. Examples includes 17 syntheses, 7 formulations, and nude mouse xenograft test results. For instance, benzylation of 1-[2-hydroxy-4-(3-chloropropoxy)-5- ethylphenyl]ethanone (69%), coupling the ethanone with 2-(3-hydroxy-2-propylphenoxy)benzoic acid Me ester (72%), oxidation to give the α-hydroxy ketone (31%), cyclization with triflic anhydride and formamide to give the oxazole (6%), debenzylation with BF3•OEt2 (45%), and deesterification (92%) afforded II (R = 4-oxazolyl). Treatment of mice with 200 mg/kg of the LTB4 antagonist, 2-[2-propyl-3-[3-[2-ethyl-5-hydroxy-4-(4-fluorophenyl)phenoxy]propoxy]phenoxy]benzoic acid (II; R = 4-FC6H4) and 50 mg/kg of carboplatin delayed growth of human H460 non-small cell lung carcinoma by an average of 33.3 days, compared to a delay of 13.9 days using the leukotriene antagonist alone or 10.7 days using carboplatin alone.

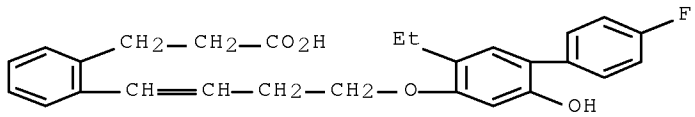
IT 152607-86-8, Methyl 3-[2-[4-[2-ethyl-4-(4-fluorophenyl)-5-hydroxyphenoxy]-1-butenyl]phenyl]propionate 185394-53-0, 3-[2-[4-[2-Ethyl-4-(4-fluorophenyl)-5-hydroxyphenoxy]-1-

butenyl]phenyl]propionic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation and use of phenoxyalkoxyphenoxybenzoic acids and analogs as leukotriene antagonists in conjunction with anti-cancer agents for treatment of cancer)

RN 152607-86-8 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]-, methyl ester (CA INDEX NAME)



RN 185394-53-0 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]- (CA INDEX NAME)



L19 ANSWER 22 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:45921 CAPLUS Full-text
DOCUMENT NUMBER: 134:105650
TITLE: Use of at least a hydroxystilbene as a glycation inhibitor in cosmetics
INVENTOR(S): Liviero, Christel; Breton, Lionel; Pageon, Herve
PATENT ASSIGNEE(S): L'oreal, Fr.
SOURCE: Eur. Pat. Appl., 10 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1068864	A1	20010117	EP 2000-401742	20000619
EP 1068864	B1	20050209		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2796278	A1	20010119	FR 1999-9267	19990716
FR 2796278	B1	20020503		
AT 288740	T	20050215	AT 2000-401742	20000619

ES 2237396	T3	20050801	ES 2000-401742		20000619
CA 2314623	A1	20010116	CA 2000-2314623		20000705
CA 2314623	C	20061114			
US 6521669	B1	20030218	US 2000-617041		20000714
JP 2001058916	A	20010306	JP 2000-216709		20000717
US 20030144363	A1	20030731	US 2002-330364		20021230
PRIORITY APPLN. INFO.:			FR 1999-9267	A	19990716
			US 2000-617041	A1	20000714

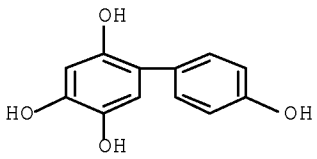
OTHER SOURCE(S): MARPAT 134:105650

AB Hydroxystilbene derivs. are used in cosmetics as inhibitors of protein glycation, especially the skin proteins. Resveratrol at 10 μM concentration decreased serum albumin glycation at 37° by 29.8%.

IT 319921-02-3, [1,1'-Biphenyl]-2,4,4',5-tetrol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(use of at least hydroxystilbene as glycation inhibitor in cosmetics)

RN 319921-02-3 CAPLUS

CN [1,1'-Biphenyl]-2,4,4',5-tetrol (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 23 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:663075 CAPLUS Full-text

DOCUMENT NUMBER: 132:22651

TITLE: Photocatalytic degradation of 4-chlorophenol. 1. The hydroquinone pathway

AUTHOR(S): Li, Xiaojing; Cubbage, Jerry W.; Tetzlaff, Troy A.; Jenks, William S.

CORPORATE SOURCE: Department of Chemistry, Iowa State University, Ames, IA, 50011-3111, USA

SOURCE: Journal of Organic Chemistry (1999), 64(23), 8509-8524
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

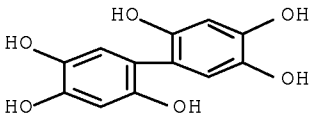
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Complete mineralization of 4-ClC6H4OH in H2O was achieved by photocatalytic degradation of oxygenated solns. containing suspended TiO2. The chemical pathways of this degradation are complex, and in this paper, that which begins with hydroquinone is examined Hydroxylation to form 1,2,4-(HO)3C6H3 (I) is the 1st step, though a very small amount of cleavage of the C1-C2 bond is observed The 1st major group of acyclic compds. derives from oxidative cleavage of either the C1-C2 or C3-C4 bond of I. This results from single-electron oxidation and capture by superoxide. Many smaller compds. were also identified, and routes to several of them are proposed. Nearly all of the compds. are verified by comparison with authentic samples.

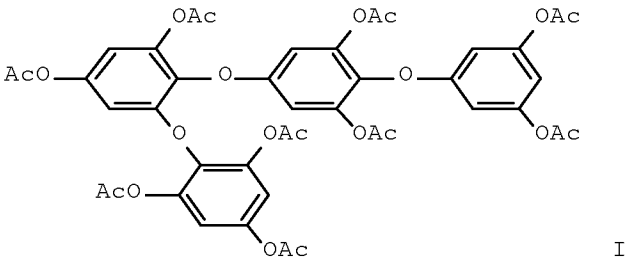
IT 76625-61-1P, 2,2',4,4',5,5'-Hexahydroxybiphenyl
RL: BYP (Byproduct); PRP (Properties); PREP (Preparation)

(hydroquinone pathway in photocatalytic degradation of chlorophenol)
RN 76625-61-1 CAPLUS
CN [1,1'-Biphenyl]-2,2',4,4',5,5'-hexol (CA INDEX NAME)



REFERENCE COUNT: 109 THERE ARE 109 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 24 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:227404 CAPLUS Full-text
DOCUMENT NUMBER: 131:41868
TITLE: Phlorethols and fucophlorethols from the brown alga Cystophora retroflexa
AUTHOR(S): Sailler, Birgit; Glombitza, Karl-Werner
CORPORATE SOURCE: Institut fur Pharmazeutische Biologie, Bonn, 53115, Germany
SOURCE: Phytochemistry (1999), 50(5), 869-881
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

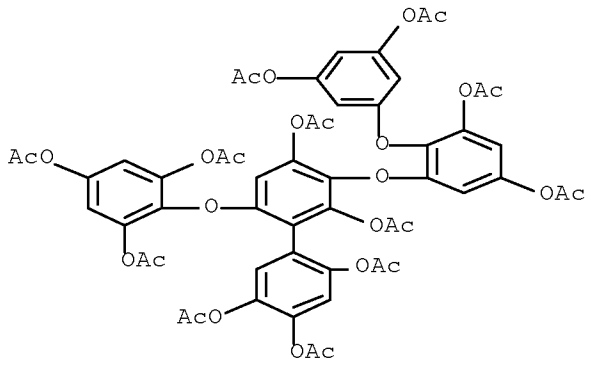
AB The ethanolic extract of the brown alga Cystophora retroflexa has yielded three different classes of phlorotannins. Most substances belong to the classes of phlorethols and fucophlorethols. Only one, well known fucol, the difucol hexa-acetate, was isolated. Three new phlorethols and ten new fucophlorethols are described and characterized as their acetates, i.e. tetraphlorethol-E nonaacetate (I), pentaphlorethol-B undecaacetate, hexaphlorethol-A tridecaacetate, fucotriphlorethol-G dodecaacetate, fucotriphlorethol-H dodecaacetate, fucotetraphlorethol-J tetradecaacetate, fucotetraphlorethol-K tetradecaacetate, fucopentaphlorethol-E hexadecaacetate, bisfucoheptaphlorethol-A tricosaacetate, difucofucotriphloretholA octadeca-

acetate, difucofucotetraphlorethol-B icosaacetate, terfucohexaphloretholB tetracosa-acetate and terfucoheptaphlorethol-A hexacosaacetate. In addition, known compds. phloroglucinol tri-acetate, diphlorethol penta-acetate, triphlorethol-A hepta-acetate, tetraphlorethol-C nona-acetate, difucol hexa-acetate, fucophlorethol-B octa-acetate, fucodiphlorethol-D deca-acetate, fucotriphlorethol-B dodeca-acetate, fucotetra-phlorethol-B tetradeca-acetate, bisfucotriphlorethol-A pentadeca-acetate, bisfucotetraphlorethol-A heptadeca-acetate, bisfucopentaphlorethol-A nonadeca-acetate, bisfucopentaphlorethol-B nonadeca-acetate, difucophlorethol-A undeca-acetate, difucofucotetraphlorethol-A icosa-acetate, terfucopentaphlorethol-A docosa-acetate and terfucohexaphlorethol-A tetracosa-acetate were identified.

IT 227085-64-5P 227085-67-8P, Difucofucotetraphlorethol B eicosaacetate 227085-69-0P, Terfucohexaphlorethol B tetracosaacetate 227085-73-6P, Terfucoheptaphlorethol A hexacosaacetate
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and mol. structure of phlorethols and fucophlorethols from the brown alga Cystophora retroflexa)

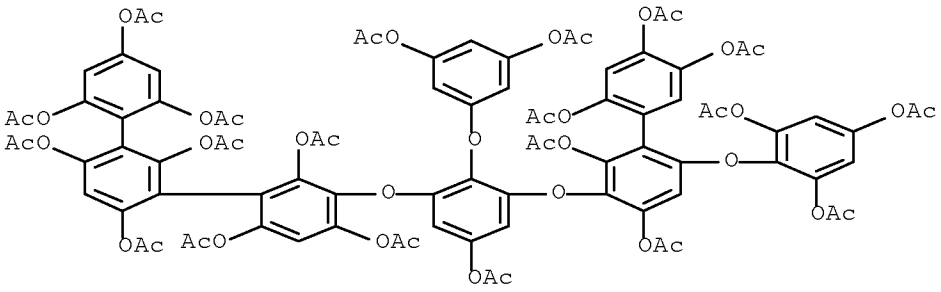
RN 227085-64-5 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4',5-pentol, 3'-[3,5-bis(acetyloxy)-2-[3,5-bis(acetyloxy)phenoxy]phenoxy]-6'-[2,4,6-tris(acetyloxy)phenoxy]-, 2,2',4,4',5-pentaacetate (CA INDEX NAME)



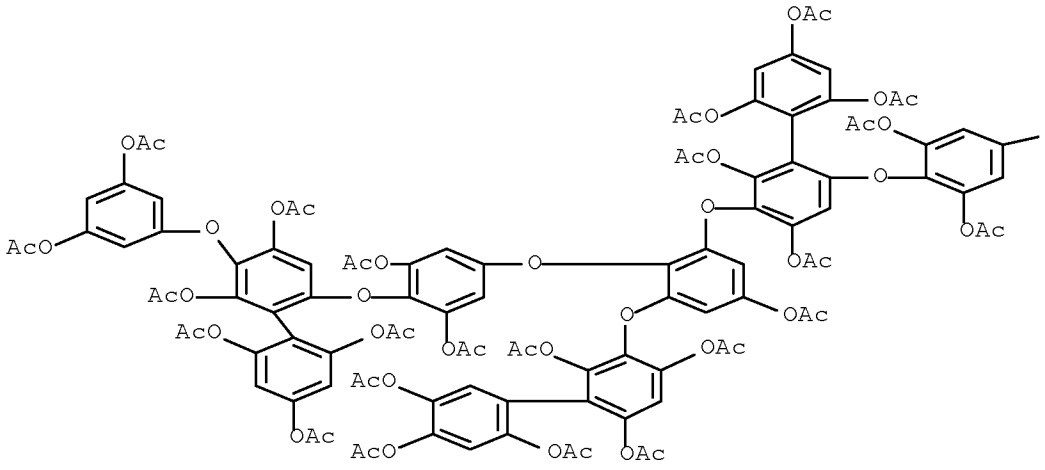
RN 227085-67-8 CAPLUS

CN [1,1':3',1''-Terphenyl]-2,2',2'',4,4',4'',6,6',6''-nonol, 3-[5-(acetyloxy)-2-[3,5-bis(acetyloxy)phenoxy]-3-[[2,2',4,4',5'-pentakis(acetyloxy)-6-[2,4,6-tris(acetyloxy)phenoxy][1,1'-biphenyl]-3-yl]oxy]phenoxy]-, nonaacetate (9CI) (CA INDEX NAME)



RN 227085-69-0 CAPLUS
CN [1,1'-Biphenyl]-2,2',4,4',5,6'-hexol, 3'-[5-(acetyloxy)-2-[3,5-bis(acetyloxy)-4-[[2',4,4',6,6'-pentakis(acetyloxy)-5-[3,5-bis(acetyloxy)phenoxy][1,1'-biphenyl]-2-yl]oxy]phenoxy]-3-[[2,2',4,4',6'-pentakis(acetyloxy)-6-[2,4,6-tris(acetyloxy)phenoxy][1,1'-biphenyl]-3-yl]oxy]phenoxy]-, hexaacetate (9CI) (CA INDEX NAME)

PAGE 1-A

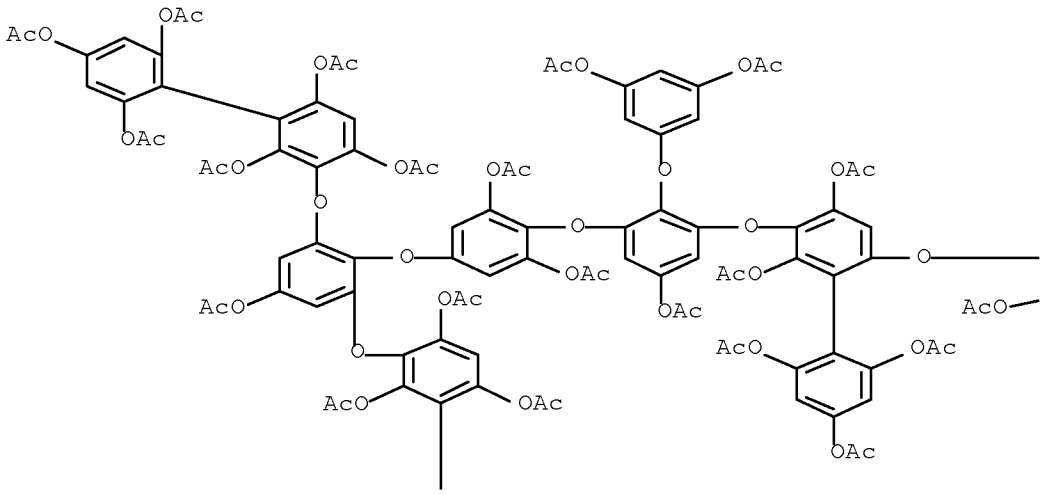


PAGE 1-B

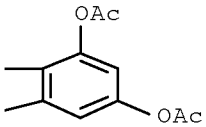
RN 227085-73-6 CAPLUS
CN [1,1'-Biphenyl]-2,2',4,4',5,6'-hexol, 3'-[5-(acetyloxy)-2-[3,5-bis(acetyloxy)-4-[5-(acetyloxy)-2-[3,5-bis(acetyloxy)phenoxy]-3-

[[2,2',4,4',6'-pentakis(acetyloxy)-6-[2,4,6-tris(acetyloxy)phenoxy][1,1'-biphenyl]-3-yl]oxy]phenoxy]phenoxy]-3-[[2,2',4,4',6,6'-hexakis(acetyloxy)[1,1'-biphenyl]-3-yl]oxy]phenoxy]- (9CI) (CA INDEX NAME)

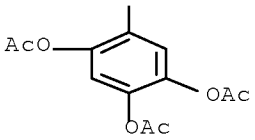
PAGE 1-A



PAGE 1-B



PAGE 2-A



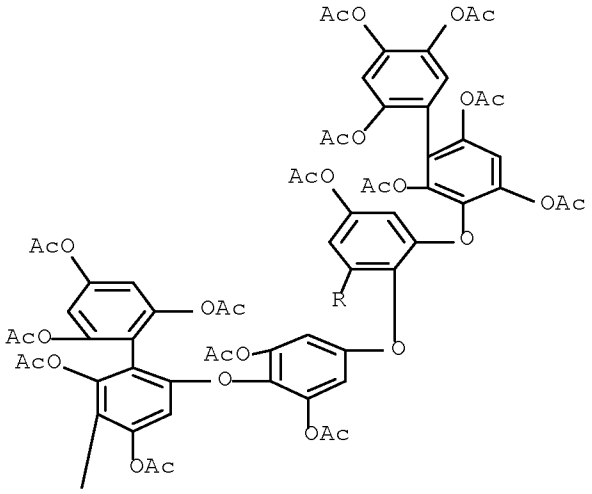
IT 227085-68-9P, Terfucopentaphlorethol A docosaacetate
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PUR

(Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and mol. structure of phlorethols and fucophlorethols from the brown alga Cystophora retroflexa)

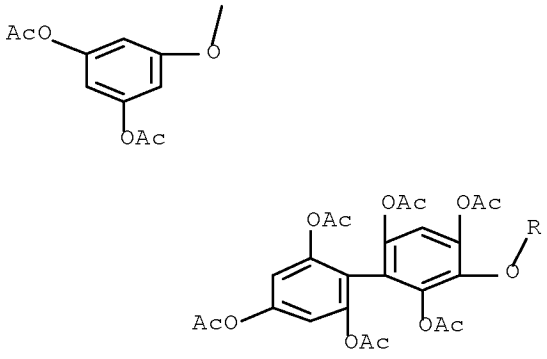
RN 227085-68-9 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4',5,6'-hexol, 3'-[5-(acetyloxy)-2-[3,5-bis(acetyloxy)-4-[[2',4,4',6,6'-pentakis(acetyloxy)-5-[3,5-bis(acetyloxy)phenoxy][1,1'-biphenyl]-2-yl]oxy]phenoxy]-3-[[2,2',4,4',6,6'-hexakis(acetyloxy)[1,1'-biphenyl]-3-yl]oxy]phenoxy]-, hexaacetate (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



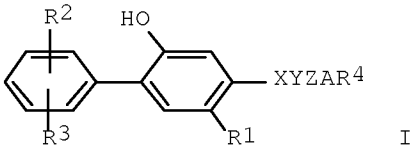
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 25 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:53684 CAPLUS Full-text
DOCUMENT NUMBER: 126:74591

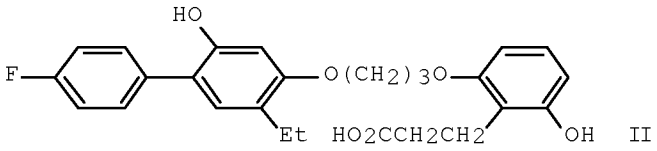
ORIGINAL REFERENCE NO.: 126:14433a,14436a
TITLE: Preparation of biphenylyloxyalkylarenes as leukotriene antagonists for the treatment or prevention of Alzheimer's disease.
INVENTOR(S): Altstiel, Larry Douglas; Fleisch, Jerome Herbert
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
SOURCE: Eur. Pat. Appl., 124 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 743064	A1	19961120	EP 1996-303346	19960513
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
WO 9636347	A1	19961121	WO 1996-US6773	19960513
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM				
RW: KE, LS, MW, SD, SZ, UG, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9658572	A	19961129	AU 1996-58572	19960513
PRIORITY APPLN. INFO.:			US 1995-443179 A	19950517
			WO 1996-US6773 W	19960513

OTHER SOURCE(S): MARPAT 126:74591
GI



I



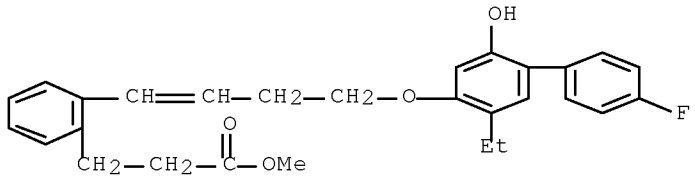
II

AB Use of compds. having leukotriene antagonist activity, e.g., title compds. [I; R1 = alkyl, alkenyl, alkynyl, alkoxy, alkylthio, halo, R2-substituted Ph; R2, R3 = H, halo, OH, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, CF3, dialkylamino; X = O, S, CO, CH2; Y = O, CH2; XY = CH:CH, C.tplbond.C; Z = alkylene; A = bond, O, S, CH:CH, etc.; R4 = (substituted) (hetero)aryl; with provisos] for manufacture of a medicament for treating or preventing Alzheimer's disease is claimed. Thus, 5-hydroxybenzopyran-2-one and 3-(2-ethyl-4-(4-fluorophenyl)-5- benzyloxyphenyl)propyl iodide were stirred with

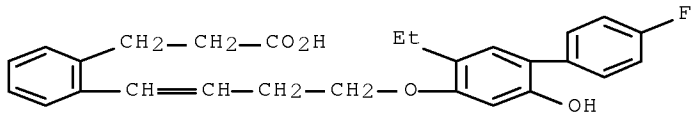
NaH in Me2SO to give 5-[3-(2-ethyl-4-(4-fluorophenyl)-5-benzyloxyphenyl)propoxy]benzopyran-2- one. This was converted to title compound (II), which displaced [3H]-LTB4 from guinea pig lung membrane prepns. with pKi = 9.01. I drug formulations are given.

IT 152607-86-8P 185394-53-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of biphenylyloxyalkylarenes as leukotriene antagonists for the treatment or prevention of Alzheimer's disease)

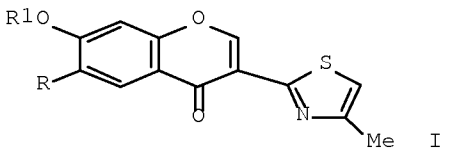
RN 152607-86-8 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]-, methyl ester (CA INDEX NAME)



RN 185394-53-0 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]- (CA INDEX NAME)



L19 ANSWER 26 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:747633 CAPLUS Full-text
DOCUMENT NUMBER: 123:339852
ORIGINAL REFERENCE NO.: 123:60995a,60998a
TITLE: Chemistry of modified flavonoids. 18. Thiazole analogs of isoflavones. Homologous and isomeric series
AUTHOR(S): Gorbulenko, N. V.; Turov, A. V.; Khilya, V. P.
CORPORATE SOURCE: Kiev. Univ., Ukraine
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1995), (4), 505-13
CODEN: KGSSAQ; ISSN: 0132-6244
PUBLISHER: Latviiskii Institut Organicheskogo Sinteza
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



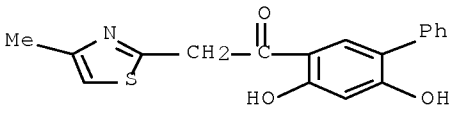
I

AB Thiazole analogs of isoflavones, e.g., I (R = alkyl; R1 = H, CHMeCOOEt), were prepared from alkyldihydroxy derivs. of α-(4-methyl-2- thiazolyl)acetophenone. The products were tested for hypolipidemic, hypoglycemic, and analeptic activity.

IT 170466-79-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(thiazole analogs of isoflavones)

RN 170466-79-2 CAPLUS

CN Ethanone, 1-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-2-(4-methyl-2-thiazolyl)- (CA INDEX NAME)



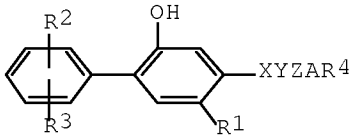
L19 ANSWER 27 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:244331 CAPLUS Full-text
DOCUMENT NUMBER: 120:244331
ORIGINAL REFERENCE NO.: 120:43289a,43292a
TITLE: Substituted phenyl phenol leukotriene antagonists
INVENTOR(S): Baker, Stephen Richard; Dillard, Robert Delane; Floreancig, Paul Edward; Sawyer, Jason Scott; Schmittling, Elisabeth Andree; Sofia, Michael Joseph
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
SOURCE: Eur. Pat. Appl., 119 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 544488	A2	19930602	EP 1992-310705	19921123
EP 544488	A3	19930728		
EP 544488	B1	19980311		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
ZA 9209051	A	19940523	ZA 1992-9051	19921123
HU 66023	A2	19940829	HU 1992-3666	19921123
HU 222486	B1	20030728		
CZ 280133	B6	19951115	CZ 1992-3460	19921123
CZ 280135	B6	19951115	CZ 1994-2766	19921123

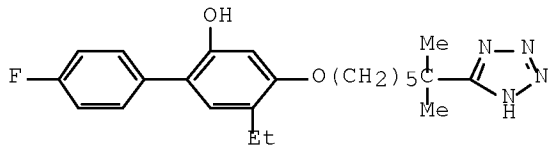
AT 163914	T	19980315	AT 1992-310705		19921123
ES 2116324	T3	19980716	ES 1992-310705		19921123
IL 116942	A	20000229	IL 1992-116942		19921123
IL 103847	A	20000601	IL 1992-103847		19921123
CA 2083639	A1	19930526	CA 1992-2083639		19921124
CA 2083639	C	20001121			
NO 9204523	A	19930526	NO 1992-4523		19921124
NO 180044	B	19961028			
NO 180044	C	19970205			
AU 9228573	A	19930527	AU 1992-28573		19921124
AU 658023	B2	19950330			
BR 9204527	A	19930720	BR 1992-4527		19921124
RU 2095340	C1	19971110	RU 1992-4509		19921124
JP 05286852	A	19931102	JP 1992-314973		19921125
JP 3417582	B2	20030616			
CN 1088906	A	19940706	CN 1993-100106		19930102
CN 1035001	C	19970528			
US 5462954	A	19951031	US 1994-333122		19941101
PRIORITY APPLN. INFO.:			US 1991-797522	A	19911125
			US 1991-797646	A	19911125
			IL 1992-103847	A3	19921123

OTHER SOURCE(S): MARPAT 120:244331

GI



I



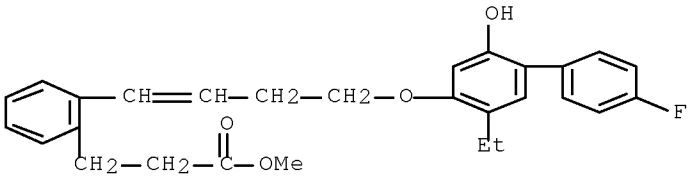
II

AB The title compds., 1,1'-biphenyl-2-ol derivs. I (R1 = alkyl, alkenyl, etc.; R2, R3 = H, alkyl, alkoxy, etc.; R4 = alkylsulfonyl, trifluoromethyl, alkylamino; X = oxygen, sulfur, methylene, carbonyl; Y = oxygen, methylene, etc.; S = bond, alkanediyl; Y = oxygen, sulfur, alkenediyl, etc.) and their uses as leukotriene antagonists are claimed. I are selective leukotriene B4 antagonists, i.e. they are useful as inflammation inhibitors, antiallergics, and antiasthmatics. Debenzylation of 2-methyl-2-(1H-tetrazol-5-yl)-7-[2-ethyl-4-(4-fluorophenyl)]-5- [(benzyloxy)phenoxy]heptane (prepared in several steps) gave 2-methyl-2-(1H-tetrazol-5-yl)-7-[2-ethyl-4-(4-fluorophenyl)]-5-hydroxyphenoxyheptane (II), [i.e. 4-ethyl-3'-fluoro-5-[[6-methyl-6-(1H-tetrazol-5-yl)heptyl]oxy]-1,1'biphenyl-2-ol]. II inhibited leukotrienes B4 in pig lung membrane with a pKi of 8.52.

IT 152607-86-8P 152607-87-9P 152608-72-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as as selective leukotriene B4 antagonist (inflammation inhibitor, antiallergic))

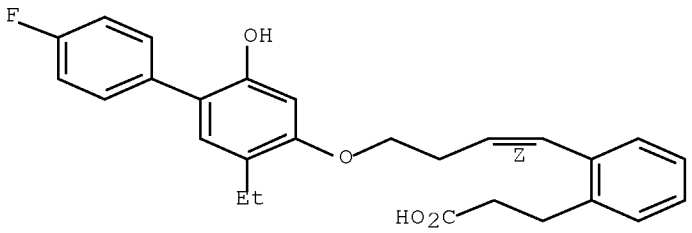
RN 152607-86-8 CAPLUS

CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-buten-1-yl]-, methyl ester (CA INDEX NAME)



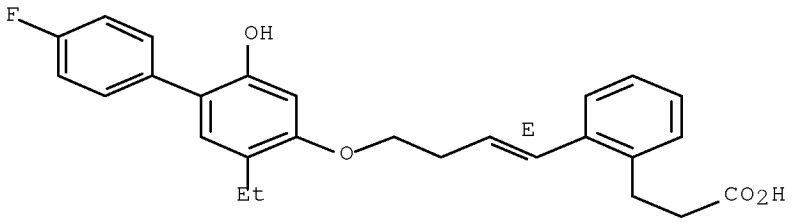
RN 152607-87-9 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-butenyl]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



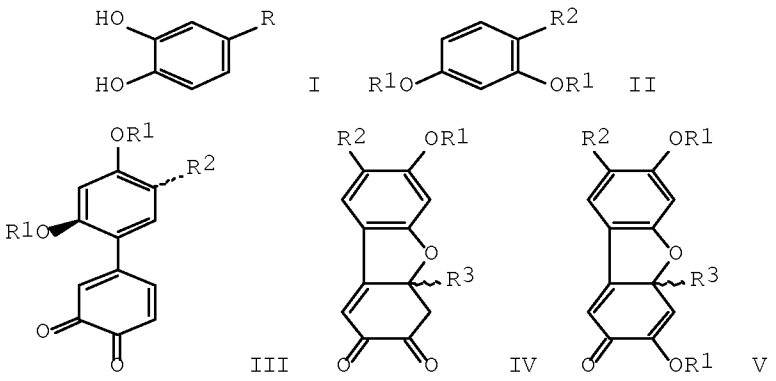
RN 152608-72-5 CAPLUS
CN Benzenepropanoic acid, 2-[4-[(5-ethyl-4'-fluoro-2-hydroxy[1,1'-biphenyl]-4-yl)oxy]-1-butenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L19 ANSWER 28 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:631969 CAPLUS Full-text
DOCUMENT NUMBER: 115:231969
ORIGINAL REFERENCE NO.: 115:39521a,39524a
TITLE: Biphenyltetrols and dibenzofuranones from oxidative coupling of resorcinols with 4-alkylpyrocatechols: new clues to the mechanism of insect cuticle sclerotization
AUTHOR(S): Miessner, Merle; Crescenzi, Orlando; Napolitano, Alessandra; Prota, Giuseppe; Andersen, Svend Olav;

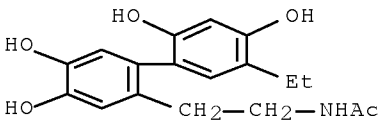
Peter, Martin G.
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300/1, Germany
SOURCE: Helvetica Chimica Acta (1991), 74(6), 1205-12
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Oxidation of 4-alkylpyrocatechols I (R = Me, AcNHCH2CH2, NH2CH2CH2CONHCH2CH2) by means of an insect diphenoloxidase (laccase) or K2[Fe(CN)6] yields, in the presence of resorcinols II (R1 = H, Me; R2 = H, Et, NH2CH2CH2, O2NCH:CH, AcNHCH2CH2), complex mixts. of products from which biphenyltetrols III and dibenzofuranones IV and V (R3 = Me, AcNHCH2CH2) were isolated. It is suggested that similar homo-coupling products are formed from pyrocatechols I (R = Me, NH2CH2CH2CONHCH2CH2) in insects during cuticle sclerotization.

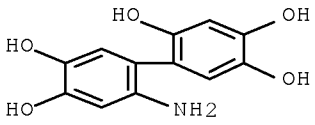
IT 136985-18-7P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in diphenoloxidase catalyzed oxidative coupling of alkylpyrocatechols with resorcinols)

RN 136985-18-7 CAPLUS
CN Acetamide, N-[2-(5'-ethyl-2',4,4',5-tetrahydroxy[1,1'-biphenyl]-2-yl)ethyl]- (CA INDEX NAME)

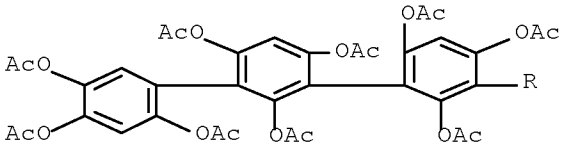


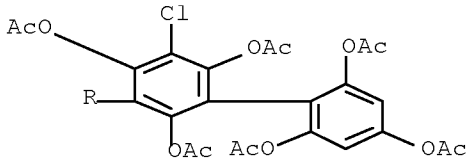
L19 ANSWER 29 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:41833 CAPLUS Full-text
DOCUMENT NUMBER: 114:41833
ORIGINAL REFERENCE NO.: 114:7281a,7284a
TITLE: Electrochemical studies on the oxidation of o-diphenols in the presence of ammonia
AUTHOR(S): Matysik, Jerzy; Przegalinski, Marek

CORPORATE SOURCE: Inst. Chem., M. Curie-Sklodowska Univ., Lublin, 20031, Pol.
SOURCE: Polish Journal of Chemistry (1990), 64(1-6), 339-44
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Oxidation by O2 of catechol in the buffer solution NH4NO3 + NH3, studied polarog., gave 2,4,5-(HO)3C6H2C6H2(OH)2NH2-4,5,2. Other products may also be present.
IT 131303-14-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 131303-14-5 CAPLUS
CN [1,1'-Biphenyl]-2,3',4,4',5-pentol, 6'-amino- (CA INDEX NAME)



L19 ANSWER 30 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:571109 CAPLUS Full-text
DOCUMENT NUMBER: 111:171109
ORIGINAL REFERENCE NO.: 111:28429a,28432a
TITLE: Antibiotics from algae. XXXIX. Phlorotannins from the brown alga Analipus japonicus
AUTHOR(S): Glombitza, K. W.; Zieprath, G.
CORPORATE SOURCE: Inst. Pharm. Biol., Univ. Bonn, Bonn, D-5300, Fed. Rep. Ger.
SOURCE: Planta Medica (1989), 55(2), 171-5
CODEN: PLMEAA; ISSN: 0032-0943
DOCUMENT TYPE: Journal
LANGUAGE: English
AB New phloroglucinol derivs. were isolated from the ethanolic extract of A. japonicus, a north Pacific brown alga. Most of the compds. are fucols, i.e. phlorotannins in which the phloroglucinol units are connected by biaryl bonds. The following were identified: difucol, trifucol, and tetrafucol A and B, 2 atropisomeric pentafucols, 4 atropisomeric hexafucols, a heptafucol mixture, bromo- and chlorotrifucol, 5'-bromo- and 5'-chlorotetrafucol-A and 5'-bromo- and 5'-chloropentafucol A. Three other phlorotannin derivs. belong to the phlorethol and fucophlorethol groups, resp.
IT 123154-77-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 123154-77-8 CAPLUS
CN [1,1':3',1'':3'',1''':3''',1''''-Quinquephenyl]-2,2',2'',2''',2'''',4,4',4'',4''',4'''',6,6',6'',6''',6''''-pentadecol, 5'-chloro-, pentadecaacetate (9CI) (CA INDEX NAME)



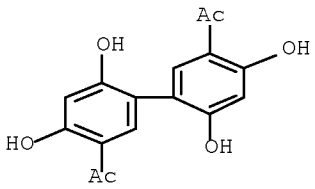


L19 ANSWER 31 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:610801 CAPLUS Full-text
DOCUMENT NUMBER: 101:210801
ORIGINAL REFERENCE NO.: 101:31931a,31934a
TITLE: Oxidative coupling of phloroacetophenone dimethyl ether, resacetophenone and resacetophenone monomethyl ether using silica-bound ferric chloride
AUTHOR(S): Parthasarathy, M. R.; Gupta, Sushma
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(3), 227-30
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English

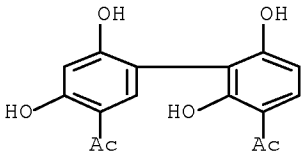
AB Oxidative C-C coupling of phloroacetophenone di-Me ether (I), resacetophenone mono-Me ether and resacetophenone with FeCl3-SiO2 yields dimers. While I affords only 1 dimer, all 3 possible dimers are obtained from the other 2 starting compds. The dimers have been converted into the biflavones by standard methods.

IT 23080-53-7P 93108-00-0P 93108-01-1P
93108-02-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

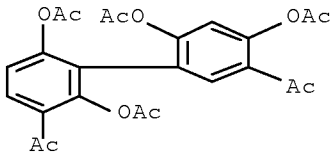
RN 23080-53-7 CAPLUS
CN Ethanone, 1,1'-(4,4',6,6'-tetrahydroxy[1,1'-biphenyl]-3,3'-diyl)bis- (9CI) (CA INDEX NAME)



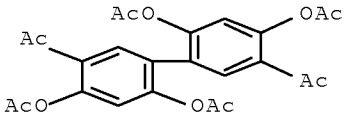
RN 93108-00-0 CAPLUS
CN Ethanone, 1,1'-(2,4',6,6'-tetrahydroxy[1,1'-biphenyl]-3,3'-diyl)bis- (9CI) (CA INDEX NAME)



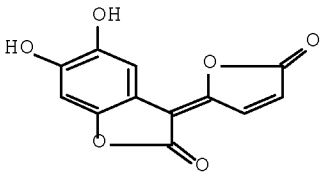
RN 93108-01-1 CAPLUS
CN Ethanone, 1,1'-[2,4',6,6'-tetrakis(acetyloxy)[1,1'-biphenyl]-3,3'-diyl]bis- (9CI) (CA INDEX NAME)



RN 93108-02-2 CAPLUS
CN Ethanone, 1,1'-[4,4',6,6'-tetrakis(acetyloxy)[1,1'-biphenyl]-3,3'-diyl]bis- (9CI) (CA INDEX NAME)



L19 ANSWER 32 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1981:476888 CAPLUS Full-text
DOCUMENT NUMBER: 95:76888
ORIGINAL REFERENCE NO.: 95:12986h,12987a
TITLE: Fungal pigments. 38. Metabolites of 1,2,4-trihydroxybenzene from fruiting bodies of Gomphidius maculatus and G. glutinosus (Boletales)
AUTHOR(S): Jaegers, Erhard; Steffan, Bert; Von Ardenne, Renata; Steglich, Wolfgang
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1981), 36C(5-6), 488-9
CODEN: ZNCBDA; ISSN: 0341-0382
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



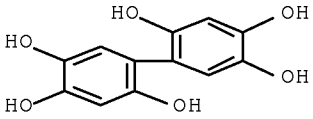
I

AB From fruiting bodies of Gomphidus 2,2',4,4',5,5'-hexahydroxybiphenyl and a red pigment, gomphilactone (I), were isolated. The latter may be derived biogenically from 1,2,4-trihydroxybenzene via oxidative dimerization to 3,5'-dihydroxydibenzoquinone followed by Posternak rearrangement.

IT 76625-61-1
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Gomphidius)

RN 76625-61-1 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4',5,5'-hexol (CA INDEX NAME)



L19 ANSWER 33 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:80497 CAPLUS Full-text

DOCUMENT NUMBER: 94:80497

ORIGINAL REFERENCE NO.: 94:13083a,13086a

TITLE: Antimicrobial metabolites of the marine sponge Axinella polycapella

AUTHOR(S): Wratten, S. J.; Meinwald, J.

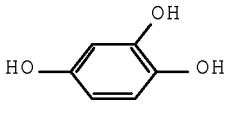
CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, USA

SOURCE: Experientia (1981), 37(1), 13-14
CODEN: EXPEAM; ISSN: 0014-4754

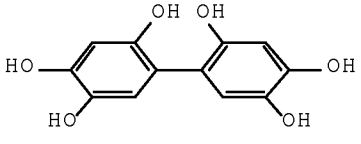
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



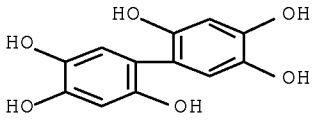
II

AB Exts. of A. polycapella contain 1,2,4-trihydroxybenzene (I) and 2,2',4,4',5,5'-hexahydroxybiphenyl (II) as antimicrobial constituents. Methods of synthesizing II by oxidative dimerization of I were examined

IT 76625-61-1
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge, bactericidal activity of)

RN 76625-61-1 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4',5,5'-hexol (CA INDEX NAME)



L19 ANSWER 34 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:423960 CAPLUS Full-text

DOCUMENT NUMBER: 89:23960

ORIGINAL REFERENCE NO.: 89:3717a,3720a

TITLE: Arylsulfonium salts

INVENTOR(S): Winkler, Adolf

PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 45 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2644591	A1	19780406	DE 1976-2644591	19761002
US 4120866	A	19781017	US 1977-833927	19770916
GB 1539481	A	19790131	GB 1977-40328	19770928
NL 7710678	A	19780404	NL 1977-10678	19770929
BE 859224	A1	19780330	BE 1977-56302	19770930
JP 53044533	A	19780421	JP 1977-117800	19770930
FR 2366273	A1	19780428	FR 1977-29553	19770930

PRIORITY APPLN. INFO.: DE 1976-2644591 A 19761002

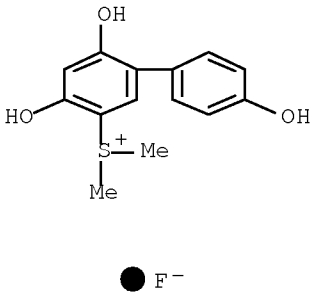
OTHER SOURCE(S): MARPAT 89:23960

AB Arylsulfonium salts were prepared by heating RH (R = aromatic, heteroarom) with R1R2SO (R1, R2 = aliphatic, aromatic; SR1R2 = heterocyclic) in HF. Thus equimolar amts. of PhMe, Me2SO and HF were heated to 70° for 10 h to give 4-MeC6H4S+Me2ClO-4, which was heated with KOH to give 4-MeC6H4SMe.

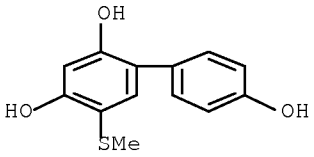
IT 66624-12-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decomposition of)

RN 66624-12-2 CAPLUS

CN Sulfonium, dimethyl(4,4',6-trihydroxy[1,1'-biphenyl]-3-yl)-, fluoride (9CI) (CA INDEX NAME)



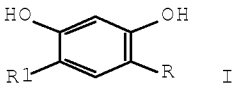
IT 66624-13-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 66624-13-3 CAPLUS
CN [1,1'-Biphenyl]-2,4,4'-triol, 5-(methylthio)- (CA INDEX NAME)



L19 ANSWER 35 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1978:152227 CAPLUS Full-text
DOCUMENT NUMBER: 88:152227
ORIGINAL REFERENCE NO.: 88:23977a,23980a
TITLE: Dihydroxybenzenes
INVENTOR(S): Kiyoura, Tadamitsu; Kogure, Yasuo
PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52151133	A	19771215	JP 1976-66417	19760609

PRIORITY APPLN. INFO.: JP 1976-66417 A 19760609
GI



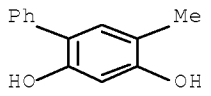
I

AB Dihydroxybenzenes I (R, R1 = H, H; Me, H; Me, Ph; resp.) were prepared by contacting MeCOCHRCH2CHR1CONH2 with dehydrogenation catalysts. Thus, 30 mL kieselguhr containing 15 weight% Ni and 5 weight% Cr was activated by passing 1:9 H-N 5 h at 400° and a 0.21 g/mL-catalyst gaseous mixture of 1:3:3.2 M MeCO(CH2)3CONH2 (II)-H-N passed 2 h at 335-40° to trap a reaction mixture of unreacted II 79, resorcinol (product) 7, dihydroresorcinol 4.2, and PhOH 1.2 weight%.

IT 66224-77-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 66224-77-9 CAPLUS

CN [1,1'-Biphenyl]-2,4-diol, 5-methyl- (CA INDEX NAME)



L19 ANSWER 36 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1976:114149 CAPLUS Full-text

DOCUMENT NUMBER: 84:114149

ORIGINAL REFERENCE NO.: 84:18480h,18481a

TITLE: Photographic material for the color diffusion transfer process

INVENTOR(S): Tsubota, Motohiko; Fuseya, Yoshiharu

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Ger. Offen., 62 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2459059	A1	19750626	DE 1974-2459059	19741213
JP 50092134	A	19750723	JP 1973-140966	19731213

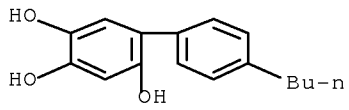
PRIORITY APPLN. INFO.: JP 1973-140966 A 19731213

AB Polyhydroxybenzenes are described for use as auxiliary developers in color diffusion-transfer photog. materials containing dye developers. These auxiliary developers, which may be incorporated into the dye-developer-containing layer, the Ag halide emulsion layer, an interlayer, or a protective layer, prevent the seepage of the dye developer into the receptor layer; hence images with a satisfactorily high maximum d. in the shadow areas and a satisfactorily low min. d. in the highlight areas can be obtained. Especially useful as an auxiliary developer is 1,2,4-trihydroxy-5-(4-butylphenyl)benzene (I), which is used with a dispersing agent, such as C6H13MeCONCH2CHMeCO2H. Thus, a cellulose acetate support coated with a cyan dye-developer layer, a red-sensitive gelatin-Ag(Br,I) emulsion layer, a gelatin interlayer containing I, a magenta dye-developer layer; a green-sensitive gelatin-Ag(Br,I) emulsion layer, a gelatin interlayer containing I; a yellow dye developer layer, a blue-sensitive gelatin Ag(Br,I) emulsion layer, and a I-containing gelatin protective layer was exposed through an optical wedge, processed with an alkali processing solution, and contacted with a receptor sheet composed of a

gelatin layer containing poly(4-vinylpyridine) and 1-phenyl-5-mercaptotetrazole on a baryta paper to give a blue-filter Dmin, a green-filter Dmin, and a red-filter Dmin of 0.38, 0.40, and 0.32, resp., vs. 0.52, 0.49, and 0.48, resp., for a I-free control.

IT 58608-08-5
RL: USES (Uses)
(photog. auxiliary developer, for color diffusion-transfer materials containing dye developers)

RN 58608-08-5 CAPLUS
CN [1,1'-Biphenyl]-2,4,5-triol, 4'-butyl- (CA INDEX NAME)

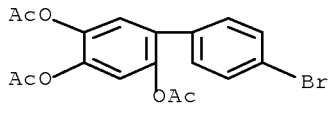


L19 ANSWER 37 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1975:155656 CAPLUS Full-text
DOCUMENT NUMBER: 82:155656
ORIGINAL REFERENCE NO.: 82:24829a,24832a
TITLE: Thiele-Winter acetoxylation of quinones. VI. Methoxy- and hydroxyphenyl-1,4-benzoquinones and (4-substituted phenyl)-1,4-benzoquinones
AUTHOR(S): Blatchly, John M.; Green, Richard J. S.; McOmie, John F. W.; Saleh, Sadig A.
CORPORATE SOURCE: Ipswich Sch., Ipswich, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1975), (4), 309-14
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

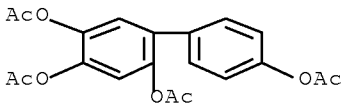
AB (Addnl. data considered in abstracting and indexing are available from a source cited in the original document). The benzoquinones I (R = MeO, OH, R1 = R2 = H, R3 = Ph; R = MeO, R1 = Ph, R2 = R3 = H; R = OH, R1 = R3 = H, R2 = Ph; R = p-O2NC6H4, p-BrC6H4, p-HOC6H4, p-AcOC6H4, R1 = R2 = R3 = H) underwent Thiele-Winter acetoxylation. The inserted AcO group always entered either ortho or para to the aryl group and never ortho to the HO or MeO group. Thus acetyoxylation of I (R = OH, R1 = R2 = H, R3 = Ph) gave 30% biphenyl II.

IT 55815-13-9P 55852-45-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

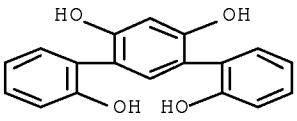
RN 55815-13-9 CAPLUS
CN [1,1'-Biphenyl]-2,4,5-triol, 4'-bromo-, triacetate (9CI) (CA INDEX NAME)



RN 55852-45-4 CAPLUS
CN [1,1'-Biphenyl]-2,4,4',5-tetrol, tetraacetate (9CI) (CA INDEX NAME)

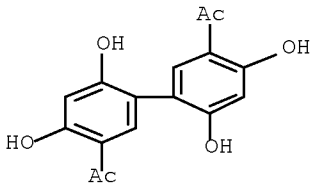


L19 ANSWER 38 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:95784 CAPLUS Full-text
DOCUMENT NUMBER: 80:95784
ORIGINAL REFERENCE NO.: 80:15403a,15406a
TITLE: Complex dibenzofurans. XIV. Acid-catalyzed demethylation and dehydration of some tetramethoxyterphenyls
AUTHOR(S): Pring, Brian G.
CORPORATE SOURCE: Res. Dev. Lab., Astra Lakemedel AB, Sodertalje, Swed.
SOURCE: Acta Chemica Scandinavica (1947-1973) (1973), 27(10), 3873-80
CODEN: ACSAA4; ISSN: 0001-5393
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The reactions of 2,4',6',2''-tetramethoxy-m-terphenyl, 2,2',5',2''-tetramethoxy-p-terphenyl (I), and 2,2',3',2''-tetramethoxy-p- terphenyl (II) with refluxing HBr were investigated. All three compds. were rapidly demethylated to the corresponding tetrahydroxyterphenyls, but only the polyphenol from I underwent facile dehydration to give first a dibenzofuran (III), then a benzobisbenzofuran (IV) as the final product. No ring-closure product was formed from II. These observations are discussed in the light of the resonance structures of the reaction intermediates.
IT 51560-18-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydration of, ring closure by)
RN 51560-18-0 CAPLUS
CN [1,1':3',1''-Terphenyl]-2,2'',4',6'-tetrol (9CI) (CA INDEX NAME)

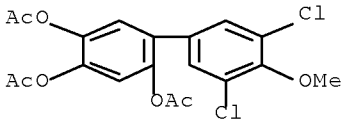


L19 ANSWER 39 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:449462 CAPLUS Full-text
DOCUMENT NUMBER: 71:49462
ORIGINAL REFERENCE NO.: 71:9073a,9076a
TITLE: Synthesis of some acetylbiphenyl derivatives and the Beckmann rearrangement of their oximes

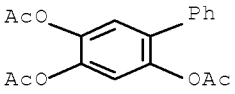
AUTHOR(S): Kanakalakshmi, B.; Sethna, Suresh
CORPORATE SOURCE: M. S. Univ. Baroda, Baroda, India
SOURCE: Journal of the Indian Chemical Society (1969), 46(5), 444-50
CODEN: JICSAH; ISSN: 0019-4522
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The Fries migration of 2,2'-diacetoxy- and 2,2'4,4'-tetraacetoxybiphenyl (I) and the Friedel-Crafts acetylation of 2,2'-dihydroxy-, 2,2',4,-4'-tetrahydroxy-, 2,2'- and 4,4'-dimethoxy, 2,2',4,4'- and 2,2',-5,5'-tetramethoxybiphenyl were studied. The acetyl derivs. were oxidized to acids of known structure. The dioximes of the diacetyl derivs. on Beckmann rearrangement with PPA [polyphosphoric acid] gave the diacetamido derivs., which on hydrolysis gave the diamino derivs., also prepared by reduction of the dinitro compds., which were prepared from the methoxybiphenyls by nitration.
IT 23080-53-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23080-53-7 CAPLUS
CN Ethanone, 1,1'-(4,4',6,6'-tetrahydroxy[1,1'-biphenyl]-3,3'-diyl)bis- (9CI) (CA INDEX NAME)



L19 ANSWER 40 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:2670 CAPLUS Full-text
DOCUMENT NUMBER: 68:2670
ORIGINAL REFERENCE NO.: 68:491a,494a
TITLE: Thiele acetylation of substituted benzoquinones
AUTHOR(S): Wilgus, Herbert S., III; Gates, John W., Jr.
CORPORATE SOURCE: Eastman Kodak Co., Rochester, NY, USA
SOURCE: Canadian Journal of Chemistry (1967), 45(17), 1975-80
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 68:2670
GI For diagram(s), see printed CA Issue.
AB The treatment of substituted quinones with (MeCO)2O under acid catalysis gives substituted triacetoxybenzenes (I). Previous work on this reaction is summarized, and the reaction was extended to include quinones having electron-withdrawing groups, and 2 quinones which were previously reported as inactive.
IT 18477-15-1P 18477-16-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 18477-15-1 CAPLUS
CN 2,4,5-Biphenyltriol, 3',5'-dichloro-4'-methoxy-, triacetate (8CI) (CA INDEX NAME)



RN 18477-16-2 CAPLUS
CN 2,4,5-Biphenyltriol, triacetate (8CI) (CA INDEX NAME)



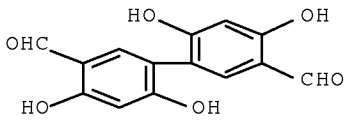
L19 ANSWER 41 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:445882 CAPLUS Full-text
DOCUMENT NUMBER: 63:45882
ORIGINAL REFERENCE NO.: 63:8237a-c
TITLE: Synthesis of resorcinol polycarbonates
AUTHOR(S): Raudsepp, H.
SOURCE: Tr. Tallinsk. Politekhn. Inst., Ser. A (1964), No. 210, 25-36
From: Ref. Zh., Khim. 1965, Abstr. No. 4S217.
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Synthesis of polyesters of carbonic acid was studied by a method of phosgenation with the use of resorcinol (I) as a model substance. The expts. were conducted to determine the suitability of the given method for preparing polycarbonates from a complex mixture of diatomic phenols from shale tar. Phosgenation was done in a solution of NaHCO3, Na2CO3(II), and NaOH, in pyridine, and in the case of heterophase polycondensation, in the presence of chlorinated or aromatic hydrocarbons (dichloromethane, chloroform, tetrachloromethane, dichloroethane, benzene, toluene, and m-xylene). I (5.506 g.) was treated with phosgene at a rate of 0.1-0.2 g./min. and the reactants mixed 15-30 min. (1-2 hrs. in the case of organic solvents); the total time was 45-60 min. (1.5-2 hrs. in the case of heterophase polycondensation). The residue was filtered off, washed with H2O, dried in air at 40-50°, and the yield of resorcinol carbonate, moisture content, m.p., and Cl and I contents were determined The highest resorcinol polycarbonate yield (90% I entered into the reaction) was obtained in a II solution at a mol. ratio of II-I of 2:1 with a 10-20% excess of phosgene. 30 references.

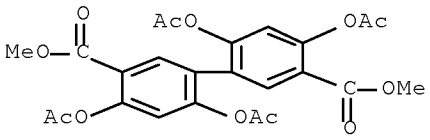
IT 2657-38-7P, 3,3'-Biphenyldicarboxaldehyde, 4,4',6,6'-tetrahydroxy-
2657-40-1P, 3,3'-Biphenyldicarboxylic acid, 4,4',6,6'-tetrahydroxy-, dimethyl ester, tetraacetate 2657-41-2P, 2,2',4,4'-Biphenyltetrol, 5,5'-dimethyl- 2811-45-2P, 3,3'-Biphenyldicarboxaldehyde, 4,4',6,6'-tetrahydroxy-, tetraacetate 2928-92-9P, 3,3'-Biphenyldicarboxylic acid, 4,4',6,6'-tetrahydroxy-, tetraacetate
RL: PREP (Preparation)
(preparation of)

RN 2657-38-7 CAPLUS

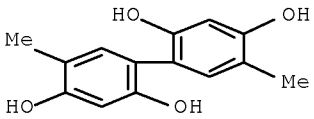
CN 3,3'-Biphenyldicarboxaldehyde, 4,4',6,6'-tetrahydro- (8CI) (CA INDEX NAME)



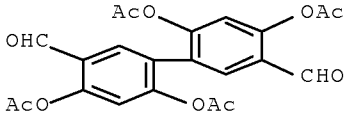
RN 2657-40-1 CAPLUS
CN 3,3'-Biphenyldicarboxylic acid, 4,4',6,6'-tetrahydroxy-, dimethyl ester, tetraacetate (7CI, 8CI) (CA INDEX NAME)



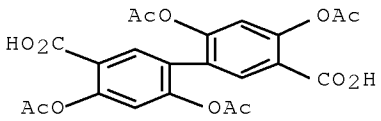
RN 2657-41-2 CAPLUS
CN [m,m'-Bitolyl]-4,4',6,6'-tetrol (8CI) (CA INDEX NAME)



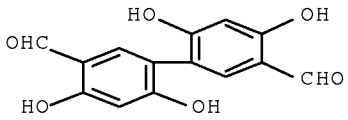
RN 2811-45-2 CAPLUS
CN [1,1'-Biphenyl]-3,3'-dicarboxaldehyde, 4,4',6,6'-tetrakis(acetyloxy)- (CA INDEX NAME)



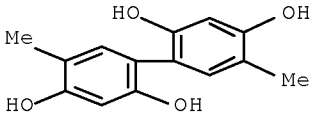
RN 2928-92-9 CAPLUS
CN [1,1'-Biphenyl]-3,3'-dicarboxylic acid, 4,4',6,6'-tetrakis(acetyloxy)- (CA INDEX NAME)



L19 ANSWER 42 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:445881 CAPLUS Full-text
DOCUMENT NUMBER: 63:45881
ORIGINAL REFERENCE NO.: 63:8236h,8237a
TITLE: The chemistry of fungi. XLVIII. Some derivatives of 2,2',4,4'-tetrahydroxybiphenyl
AUTHOR(S): ApSimon, J. W.; Creasey, N. G.; Marlow, W.; Sim, K. Y.; Whalley, W. R.
CORPORATE SOURCE: Univ. London
SOURCE: Journal of the Chemical Society (1965), (July), 4156-63
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. CA 63, 6956f. Syntheses are described of various 3-acetyl-, 3-ethyl-, 3,3'-diacetyl-, and 3,3'-diethyl-2,2',4,4'-tetrahydroxybiphenyls, including those obtained as degradation products from the ergot pigments, ergoflavin and ergochrysin.
IT 2657-38-7P, 3,3'-Biphenyldicarboxaldehyde, 4,4',6,6'-tetrahydroxy-
2657-41-2P, 2,2',4,4'-Biphenyltetrol, 5,5'-dimethyl-
2811-45-2P, 3,3'-Biphenyldicarboxaldehyde, 4,4',6,6'-tetrahydroxy-, tetraacetate
RL: PREP (Preparation)
(preparation of)
RN 2657-38-7 CAPLUS
CN 3,3'-Biphenyldicarboxaldehyde, 4,4',6,6'-tetrahydro- (8CI) (CA INDEX NAME)

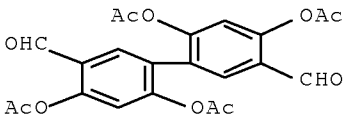


RN 2657-41-2 CAPLUS
CN [m,m'-Bitolyl]-4,4',6,6'-tetrol (8CI) (CA INDEX NAME)



RN 2811-45-2 CAPLUS

CN [1,1'-Biphenyl]-3,3'-dicarboxaldehyde, 4,4',6,6'-tetrakis(acetyloxy)- (CA INDEX NAME)



L19 ANSWER 43 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:492144 CAPLUS Full-text
DOCUMENT NUMBER: 61:92144
ORIGINAL REFERENCE NO.: 61:16008a-h
TITLE: Formation of hydroxy aryl quinones by the addition of phenols to quinones
AUTHOR(S): Musso, Hans; Gizycki, Ulrich v.; Zahorszky, Uwe I.; Bormann, Dieter
CORPORATE SOURCE: Univ. Marburg, Germany
SOURCE: Justus Liebigs Annalen der Chemie (1964), 676, 10-20
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 61:92144
GI For diagram(s), see printed CA Issue.

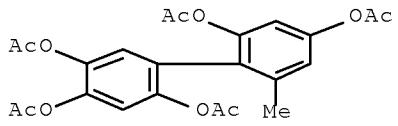
AB Resorcinol derivs. add in alkaline solution to hydroxyquinones to yield the corresponding dihydroxyarylhydroquinones. PHOH reacts in acidic and alkaline solution with p-benzoquinone (I) to give o-(II) and p-hydroxyphenylbenzoquinone (III); in neutral solution phenoxyquinones are also formed. The condensation of hydroxy-p-xyloquinone (IV) with BF3 led to a dibenzofuranquinone, present in nonpolar solvents as diphenoquinone. m-C6H4(OH)2 (1 g.) in 25 cc. 0.2M phosphate buffer (pH 12) and 4 cc. 2N NaOH treated dropwise with stirring in air with 100 mg. 1,2,4-C6H3(OH)3 in 10 cc. H2O and acidified after 20 min. with dilute H2SO4, and the crude product chromatographed on silica gel yielded 38 mg. V (R = R1 = R2 = R3 = H) (VI), dark brown needles, blacken up to 320° without melting. Similarly were prepared the following V (R, R1, R2, R3, % yield, and m.p. given): Me, H, Me, H, 92.5, 182-7° (decomposition); Me, Me, Me, Me, 90, 224-5°; tert-Bu, H, tert-Bu, H, 39.5, 225-7° (orange needles) (AcOEtcyclohexane); H, H, Me, H, 28, 190-200° (decomposition); Me, H, H, H, 11, 180-200° (decomposition). VI (125 mg.) in 5 cc. Ac2O heated 0.5 hr. on the water bath with NaOAc and Zn dust, and the product chromatographed on silica gel yielded 207 mg. 2,2',4,4',5-pentaacetoxybiphenyl (VII), m. 123-4° (cyclohexane-C6H6). Similarly were prepared the following derivs. of VII (substituent, % yield, and m.p. given): 6'-Me, 68, 136-9°; 6-Me, 84, 133-4°. 6-Hydroxytoluhydroquinone (141 mg.) in 25 cc. 0.2M phosphate buffer (pH 12) stirred 1 hr. in air and acidified with dilute H2SO4, and the product chromatographed on silica gel yielded 91 mg. 4,4'-dihydroxy-2,2'- ditolyldiquinone, yellow needles, m. 207°. Similarly was prepared 4,4'-dihydroxy-3,3',6,6'-tetramethylbiphenyldiquinone, 68%, m. 208-10°. PhOH (5.64 g.) and 1.58 g. KOH in 20 cc. H2O treated with stirring with 0.648 g. I in 20 cc. H2O and acidified after 4 min. with dilute H2SO4, and the product chromatographed on silica gel yielded 5 mg. 5-PhO derivative (VIII) of 2-(p-hydroxyphenoxy)-1,4-benzoquinone (IX), light yellow needles, m. 224-6°, and 43 mg. III, m. 177° (C6H6-cyclohexane). PhOH (5.64 g.) in 35 cc. 20% H2SO4 and 7 cc. MeOH treated 0.5 hr. at 40° with 0.65 g. I yielded 103 mg. II, m. 192-3°, and 10 mg. III. I (3g.) and 18 g. PhOH in 850 cc. H2O and 150 cc. MeOH kept 20 days, and the crude product chromatographed on silica gel yielded

170 mg. yellow 2,5-diphenoxy-1,4-benzoquinone, m. 236-7° (cyclohexane), 95 mg. X, 220 mg. IX, 100 mg. VIII, yellow needles, m. 224-6° (AcOEt-cyclohexane), and 1.5 g. p-C6H4(OH)2. VIII (20 mg.) with 5 cc. Ac2O and 1 cc. C5H5N yielded 17 mg. acetate of VIII, yellow-green needles, m. 192-4° (C6H6). VIII (27 mg.) in 10 cc. Ac2O treated with 2 g. Zn dust yielded 22 mg. 2-(p-acetoxyphenoxy)-5-phenoxyhydroquinone diacetate, m. 102° (C6H6-cyclohexane). I (2 g.) in 200 cc. H2O and 25 cc. MeOH kept 9 days and acidified with dilute H2SO4 yielded 25 mg. IX, yellow needles, m. 145-6° (C6H6-cyclohexane). IX (216 mg.) and 2 g. PhOH in 150 cc. H2O and 25 cc. MeOH kept 13 days yielded 25 mg. VIII, yellow needles, m. 224-6° (AcOEt-cyclohexane). II (100 mg.) in 30 cc. dry Et2O treated 2 hrs. with 0.5 cc. Et2O.BF3 yielded 80 mg. 1,4,5,8-tetramethyl-3,6-dihydroxydibenzofuran-2,7-quinone (XI), black-blue needles, decompose slowly above 300° without melting up to 350° (AcOEt). II (150 mg.) in 15 cc. AcOH treated 4 hrs. at room temperature with 0.5 cc. concentrated H2SO4 gave 102 mg. XI. XI (100 mg.) and a small amount NaOAc in 5 cc. Ac2O heated with the portionwise addition of 3 g. Zn dust until the mixture was colorless gave 116 mg. 1,4,5,8-tetramethyl-2,3,6,7-tetraacetoxydibenzofuran (XII), needles, m. 275-6° (C6H6). 2,7-Dihydroxy-4,5-dimethyldibenzofuran (30 mg.) in 10 cc. Ac2O and 1 cc. C5H5N heated 15 min. on the water bath, and the crude product chromatographed on silica gel yielded 34 mg. diacetate, needles, m. 181-2° (C6H6-cyclohexane). XI (100 mg.) in 100 cc. Me2CO and 5 cc. 2N HCl shaken with Zn dust until colorless gave 30 mg. 2,3,6,7-tetra-OH analog (XIII) of XII, needles, m. 285-300° (decomposition). The ultraviolet spectra of XI and XIII are recorded.

IT 107893-61-8P, 2,2',4,4',5-Biphenylpentol, 6'-methyl-, pentaacetate
RL: PREP (Preparation)
(preparation of)

RN 107893-61-8 CAPLUS

CN 2,2',4,4',5-Biphenylpentol, 6'-methyl-, pentaacetate (7CI) (CA INDEX NAME)



L19 ANSWER 44 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1964:2878 CAPLUS Full-text

DOCUMENT NUMBER: 60:2878

ORIGINAL REFERENCE NO.: 60:440b-c

TITLE: Thiele acetylation of 2-phenyl-1,4-benzoquinone and its 5 methoxy derivative

AUTHOR(S): Blatchly, J. M.; McOmie, J. F. W.

CORPORATE SOURCE: Univ. Bristol, UK

SOURCE: Journal of the Chemical Society (1963), (Nov.), 5311-13
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

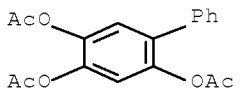
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

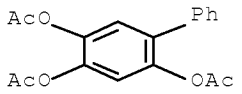
AB The products from Thiele acetylation of 2-phenyl-1,4-benzoquinone (I) and its 5-methoxy derivative have been shown to be 2,4,5-triacetoxybiphenyl (II) and 2,3,6-triacetoxy-4-methoxy biphenyl, resp. Three other similar quinones did not undergo Thiele acetylation.

IT 18477-16-2P, 2,4,5-Biphenyltriol, triacetate

RL: PREP (Preparation)
(preparation of)
RN 18477-16-2 CAPLUS
CN 2,4,5-Biphenyltriol, triacetate (8CI) (CA INDEX NAME)



L19 ANSWER 45 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:2877 CAPLUS Full-text
DOCUMENT NUMBER: 60:2877
ORIGINAL REFERENCE NO.: 60:439g-h,440a-b
TITLE: Alkylaminomethylhydroquinones and related compounds
AUTHOR(S): Weatherbee, Carl; Lau, Howard K. S.; Snell, Robert; Goken, Garold; Van Lear, George
CORPORATE SOURCE: Millikin Univ., Decatur
SOURCE: Transactions of the Illinois State Academy of Science (1963), 56(1), 12-18
CODEN: TISAAH; ISSN: 0019-2252
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 56, 15504d. Condensation of PhCH2NH2 (I) and (PhCH2)2NH (II) with CH2O (III) in the presence of p-benzyloxyphenol (IV) and hydroquinone (V) was studied. To 30.6 ml. 40% III in PrOH and 50 ml. dioxane was added with stirring during 3-4 min. at 10-15° 22 ml. I, followed by 40 g. IV and 25 ml. dioxane. After being stirred until homogeneous, refluxed 2 hrs., allowed to stand 22 hrs. at 25°, and evaporated, the mixture gave a solid which was dissolved in 300 ml. Et2O and 150 ml. H2O containing 11 g. NaOH. The Et2O layer gave 57 g. crude 3,4-dihydro-3-benzyl-6-benzyloxy- 2H1,3-benzoxazine (VI), m. 86-7° (2:5 MeOH-EtOH). Similarly, 2-benzylaminomethyl-4-hydroxyphenol (VII) was converted in 91.5% yield to 3,4-dihydro-3-benzyl-6-hydroxy-2H-1,3-benzoxazine, m. 105-6° (CCl4). A solution of 3.6 g. VI and 3 ml. concentrated HCl in 25 ml. EtOH was distilled until 15 ml. EtOH (and III) was removed, and the residue was cooled and treated with 20 ml. acetone to give 3.4 g. 2-benzylaminomethyl-4- benzyloxyphenolHCl (VIII), m. 170-1° (EtOH). A stirred mixture of 4.95 g. VIII and 1.5 ml. HOCH2CH2NH2 in 150 ml. H2O was extracted with Et2O to give 4.16 g. 2-benzylaminomethyl-4-benzyloxyphenol (IX), m. 90-1° (MeOH). To a solution of 6.39 g. IX in 100 ml. MeOH was added to 0° 1.5 ml. 37% aqueous III, and the mixture refluxed 2 hrs. to give 5.3 g. VI. Refluxing 30 min. a mixture of 8.8 g. IX and 15 ml. concentrated HCl gave 5.1 g. 2-benzylaminomethylhydroquinoneHCl (X), m. 177-8° (iso-PrOH). IV was similarly cleaved to V. An aqueous solution of X was saturated with KHCO3 and extracted with Et2O to give VII, m. 120-20.5° (C6H6). Attempted condensations of II, III, and either IV or V under a variety of conditions led to 96100% tetrabenzyldiaminomethane (XI). XI did not react further with III and IV. Neither I nor I.HCl would react with III and V.
IT 18477-16-2P, 2,4,5-Biphenyltriol, triacetate
RL: PREP (Preparation)
(preparation of)
RN 18477-16-2 CAPLUS
CN 2,4,5-Biphenyltriol, triacetate (8CI) (CA INDEX NAME)



L19 ANSWER 46 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:15521 CAPLUS
DOCUMENT NUMBER: 56:15521
ORIGINAL REFERENCE NO.: 56:2914a-b
TITLE: Hardening of gelatin films, especially photographic emulsions
INVENTOR(S): Joachim Birr, Emil; Walther, Werner
PATENT ASSIGNEE(S): VEB Filmfabrik Agfa Wolfen
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1112282		19610803	DE 1959-V15860	19590130

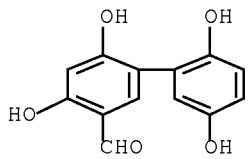
PRIORITY APPLN. INFO.: DE 19590130

AB Small amts. of compds. containing 2 hydroxylated phenyl moieties speed the hardening of photographic emulsions. These compds. include 2,2',4,5'-tetrahydroxybiphenyl (I); 2',3,4,5'-tetrahydroxybiphenyl (from pyrocatechol and quinone); 3,3',4,4'-tetrahydroxydiphenylmethane (from pyrocatechol and acetone in the presence of HCl, m. 284-6°); 3,3',4,4'-tetrahydroxy5,5'-disulfodiphenylmethane; 3,3',4,4'- tetrahydroxydiphenylmethanol; 2,2',4,5'-tetrahydroxy-5'-formylbiphenyl (from I and Zn(CN)2 in the presence of HCl followed by treating the imide hydrochloride with H2SO4, m. 172°); 2',3,4,5'tetrahydroxy-5- formylbiphenyl; and 2,2',4,4'-tetrahydroxydiphenyl sulfone, from H2O2 oxidation of the sulfide.

IT 92379-40-3, 3-Biphenylcarboxaldehyde, 2',4,5',6-tetrahydroxy- (photographic-emulsion hardening by)

RN 92379-40-3 CAPLUS

CN β-Resorcylaldehyde, 5-(2,5-dihydroxyphenyl)- (7CI) (CA INDEX NAME)



L19 ANSWER 47 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:5953 CAPLUS
DOCUMENT NUMBER: 56:5953
ORIGINAL REFERENCE NO.: 56:1093d-f
TITLE: Hardeners for photographic emulsions
INVENTOR(S): Birr, Emil Joachim; Walther, Werner
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable

PATENT INFORMATION:

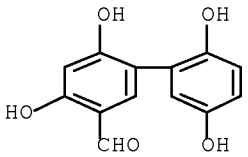
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 20032		19590113	DD	

AB Hardening accelerators are described, e.g. polyphenols, which intensify and speed up the hardening of gelatin photographic emulsions (by using diacetyl as hardener) and prevent posthardening. Fusing 22 g. pyrocatechol (I) with 21.6 g. quinone, heating is for 30 min., and extracting with C6H6 gives 2',3,4,5'-tetrahydroxybiphenyl (II). The 2,2',4,5'isomer (III) of II, 109 g., prepared from resorcinol and quinone, in 600 ml. ether is treated with 88 g. anhydrous Zn(CN)2, cooled, stirred, and saturated with HCl gas. The ether is decanted from the imido chloride formed and the latter decomposed with 10% aqueous H2SO4 to give the 5-formyl derivative of III, m. 172°. Refluxing 29 g. I in 7.2 acetone and 20 ml. concentrated HCl for 6 hrs. and washing the product with hot water gives 2,2-bis(3,4- dihydroxyphenyl)propane (IV), m. 284-6°. A similar treatment of pyrocatecholsulfonic acid or sulfonation of IV with aminosulfonic acid yields the 5-sulfo derivative Tests are reported with 1-1. portions of an NH3-AgBr plus AgClgelatin emulsion by using 0.33 or 0.66 g. diacetyl and 0.13 g. accelerator to effect hardening.

IT 92379-40-3, 3-Biphenylcarboxaldehyde, 2',4,5',6-tetrahydroxy- (photographic-emulsion hardening by)

RN 92379-40-3 CAPLUS

CN β-Resorcylaldehyde, 5-(2,5-dihydroxyphenyl)- (7CI) (CA INDEX NAME)



L19 ANSWER 48 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:27751 CAPLUS Full-text

DOCUMENT NUMBER: 50:27751

ORIGINAL REFERENCE NO.: 50:5559g-i,5560a

TITLE: Antiseptics for foods. LVIII

AUTHOR(S): Fujikawa, Fukujiro; Tokuoka, Akimasa; Nishimoto, Masaharu; Miura, Kazuko

CORPORATE SOURCE: Kyoto Coll. Pharm.

SOURCE: Yakugaku Zasshi (1955), 75, 600-2
CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

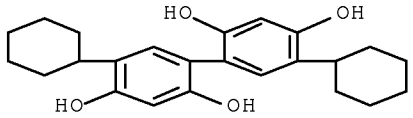
AB cf. C.A. 49, 11596i. 4,1,3-C6H11C6H3(OMe)2 (2.2 g.) in 50 ml. Et2O and 3 g. iodine treated with 1.5 g. HgO with shaking 7 hrs., filtered, the filtrate washed with 7% NaHSO3, 20% KI, and 5% KOH, the Et2O removed, and the residue recrystd. from ligroine gives 6,4,1,3-I(C6H11)C6H2(OMe)2 (I), columns, m. 133°; 9 g. I and 22.5 g. Cu powder in a sealed tube heated several hrs. at 210-20°, and the product extracted with Me2CO and recrystd. from ligroine gives [3,4,6-C6H11(MeO)2C6H2]2 (II), columns, m. 146°; 1 g. II, 20 ml. AcOH and 10 ml. HI boiled and the product recrystd. from dilute EtOH give [3,4,6-C6H11(HO)2C6H2]2, columns, m. 267°. 3,2,4,5-Cl(HO)2(iso-Am)C6HCHO (?g.), 43 ml. concentrated HCl, 40 ml. water, 30 ml. PhMe and 30 g. Zn-Hg heated 5 hrs. on an oil bath, the PhMe removed, the residue extracted with Et2O, the extract

washed with 10% NaOH, the Et2O removed, and the residue recrystd. from dilute EtOH give 2,6,4,1,3-ClMe(iso-Am)C6H(OH)2, columns, m. 102°. Similarly, 3,5,2,4-Cl[Me(CH2)5](HO)2C6HCHO gives 2,6,4,1,3-ClMe(C6H13)C6H(OH)2, columns, m. 73°. Me agaricate (0.4 g.) in 5 ml. EtOH heated 5 min. on a water bath with 0.45 g. N2H4.H2O and the product recrystd. from EtOH gives agaricic acid trihydrazide, m. 170° (decomposition). The above compds. and quinoxaline, pyrazinecarboxylic acid (III), 2,3-pyrazinedicarboxylic acid (IV), nicotinic acid (V), and the corresponding Me esters and acid hydrazides of III, IV, and V were tested for mold-preventing action on soy sauce but none of them showed any marked action up to a concentration of 0.01%.

IT 873996-64-6P, 2,2',4,4'-Biphenyltetrol, 5,5'-dicyclohexyl-
RL: PREP (Preparation)
(preparation of)

RN 873996-64-6 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 5,5'-dicyclohexyl- (CA INDEX NAME)



L19 ANSWER 49 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1954:1175 CAPLUS Full-text

DOCUMENT NUMBER: 48:1175

ORIGINAL REFERENCE NO.: 48:229f-i,230a

TITLE: Antibacterial activity of some organic compounds in vitro. II. Antibacterial activity of some organic compounds on Micrococcus pyogenes var. aureus, Escherichia coli communior, and Bacillus subtilis

AUTHOR(S): Fujikawa, Fukujiro; Hitosa, Yuhei; Yamaoka, Michiyo; Fujiwara, Yoshiko; Nakazawa, Shozo; Omatsu, Tokugoro; Toyoda, Tadaaki

SOURCE: Yakugaku Zasshi (1953), 73, 135-8
CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

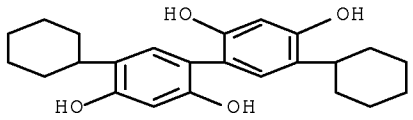
AB The growth-inhibitory action of the following compds. was tested on M. pyogenes var. aureus, E. coli communior, and B. subtilis, in the order named, and the effective dilns. (10,000 dilution = 1) were: (2-HOC6H4)2O, 1, 1, and <1; 2-HOC6H4OC6H4OH-4, 1, 1, and <1; (4-HOC6H4)2O, 1, 1, and 1; 2-HOC6H4OC6H4Me-2, 2, 2, and 1; 2-HOC6H4OC6H4Me-4, 4, 1, and 1; 3-MeC6H4OC6H3(OH)2-2, 5, 4, 1, and 2; 2,5-(HO)2C6H3OC6H4Me-4, 2, 1, and 2; 2,5-Me2C6H3OC6H4OH-4, 8, <1, and 2; 2,4,6-Me(HO)2C6H2OC6H4Me-4, 1, <1, and <1; 2,5,3-Me2(HO)C6H2OPh, 2, 1, and 8; 2,5,3-Me2(HO)C6H2OC6H4OH-2, 1, 1, and 1; 2,5,4,6-Me2(HO)2C6HOC6H4Me-2, 2, 1, and 2; 2,5,4,6- Me2(HO)2C6HOC6H4Me-3, 1, <1, and 1; 2,5,4,6-Me2(HO)2C6HOC6H4Me-4, 1, <1, and 1; 2-HO2CC6H4OPh, 1, 1, and <1; 3-HO2CC6H4OPh, all <1; 2-HOC6H4OC6H4CO2H-2, all <1; 3-HOC6H4OC6H4CO2H-3, 1, 1, and <1; 3-HO2CC6H4OC6H4OH-4, all <1; 3-HO2CC6H4OC6H4OMe-4, all <1; PhOC6H3(OH)CO2H-3,5, all <1; 2-HO2CC6H4OC6H4CO2H-4, all <1; 3,5-HO(HO2C)C6H3OC6H4CO2H-4, all <1; 4-ClC6H4OC6H4OMe-4, all 1; 4-ClC6H4OC6H4OH-4, all 1; (2-HOC6H4)2, all 1; [2,4-(HO)2C6H3]2, 1, 1, and <1; [2,4,6-Me(MeO)2C6H2]2, all <1; [2,4,6-Me(HO)2C6H2]2, 2, 1, and <1; [2,4,5-(HO)2RC6H2]2, R = cyclohexyl, 1, <1, and 1; (4-HO2CC6H4)2, all <1; [2,5,4,6-Me2(HO)2C6H]2, all <1; 2,7-dimethoxy-4,5-dimethyldiphenylene oxide, all <8; 2,7-dihydroxy-4,5-dimethyldiphenylene oxide, <8, <8, and 16; 2,7-

dihydroxydiphenylene oxide 4,5-dicarboxylic acid, all <8; the Me ester of the latter, all <8; divaricatic acid, 2, <1, and 16; atranorin, <1, 1, and <1; sekikaic acid, 1, <1, and 4; sphaerophorin, 1, <1, and 16; gyophoric acid, all <8; anziaic acid, all 8; microphyllic acid, all 8; Me lecanorate, all <1; protocetraric acid, all 8; α-collatolic acid, all 8; β-collatolic acid, <8, 8, and <8; collatolon, 16, 8, and <8; stictinic acid, <8, 8, and <8; psoromic acid, all <1; usnolic acid, all <1; Et usnolate, 2, 4, and 4; usnetol, all <1; rangiformic acid, 8, 8, and <8; l-protolichesterinic acid, 8, <1 and 1; agaricinic acid, 1, 1, and <1; sphaerophorol, 8, 1, and 8.

IT 873996-64-6, 2,2',4,4'-Biphenyltetrol, 5,5'-dicyclohexyl-
(as bactericide)

RN 873996-64-6 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4'-tetrol, 5,5'-dicyclohexyl- (CA INDEX NAME)



L19 ANSWER 50 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1953:34889 CAPLUS Full-text

DOCUMENT NUMBER: 47:34889

ORIGINAL REFERENCE NO.: 47:5917a-c

TITLE: Inhibition of hyaluronidase by gentisic acid and its oxidation products

AUTHOR(S): Forrest, J.; Overell, B. G.; Petrow, V.; Stephenson, O.

CORPORATE SOURCE: Brit. Drug Houses, Ltd., London

SOURCE: Journal of Pharmacy and Pharmacology (1952), 4, 231-42
CODEN: JPPMAB; ISSN: 0022-3573

DOCUMENT TYPE: Journal

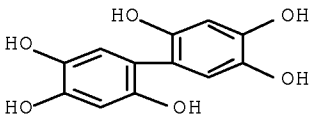
LANGUAGE: Unavailable

AB cf. Roseman, et al., Federation Proc. 8, 245(1949). Oxidation of C6H4(OH)CO2H with (NH4)2S2O8, extraction, and purification yields compound A as an amorphous black solid (C6H4O3), m. about 240° (decomposition), which inhibits the action of hyaluronidase (I) on hyaluronic acid. Aerial oxidation of Me gentisate with p-quinone in alkaline solution gave, on addition of HCl, compound B as a black infusible solid which inhibited I. Compound C was obtained from pyrocatechol. C6H3(OAc)3 hydrolyzed with 10% H2SO4 then mixed with a p-quinone suspension in 10% H2SO4 gave 2,2',4,4',5,5'-hexahydroxybiphenyl, C12H10O6, a light blue-gray solid, m. 277-80°. Alkaline aeration of nitrohydroquinone yields, from AcOEt-light petr., small bright red needles of 2,2',5,5'-tetrahydroxy-3,3'-dinitrophenyl, C12H8O8N2 m. 240° (decomposition); tetra-AcO analog, m. 191°. 2,2',3,3'-Tetrahydroxy-5,5'-dinitrobiphenyl, from nitropyrocatechol, forms brown microcrystals, m. above 300° (decomposition); tetraacetate, m. 170°. Other compds. aerated alone or with hydroquinone or p-quinone in alkaline media yielded dark products that showed inhibitory action. Comparison of the inhibiting products with humic acid from soil and peat indicate that the oxidation products are of the humic acid type. The natural humic acids are also inhibitors of the action of I.

IT 76625-61-1, 2,2',4,4',5,5'-Biphenylhexol
(and inhibiting action on hyaluronidase)

RN 76625-61-1 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4',5,5'-hexol (CA INDEX NAME)

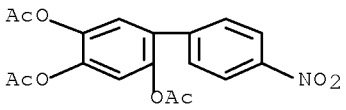


L19 ANSWER 51 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1943:552 CAPLUS Full-text
DOCUMENT NUMBER: 37:552
ORIGINAL REFERENCE NO.: 37:109h-i,110a-d
TITLE: The action of diazo compounds on quinones. The preparation of some derivatives of biphenyl
AUTHOR(S): Marini-Bettolo, G. B.
SOURCE: Gazzetta Chimica Italiana (1941), 71, 627-35
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

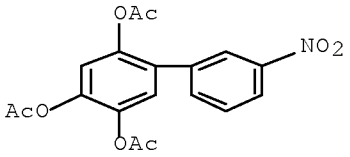
AB Condensation of diazotized m- and p-O2NC6H4NH2 (I and II) with quinone (III) forms the corresponding nitrophenyl-quinones. Some reduction products and derivs. of these are described. II (14 g.), diazotized, and condensed with 10.8 g. III in the presence of 30 g. NaOAc, first at 0°, then at room temperature, and the product purified by AcOH, yields p-nitrophenylquinone (IV), brown, m. 135°. IV (1 g.) and SO2 in boiling water form 4-nitro-3',6'-dihydroxybiphenyl (V), orange-yellow, m. 195°. Alc. V, 8 mols. Me2SO4 and 33% aqueous KOH yield, after purification of the product from EtOH, 4-nitrodimethoxybiphenyl (VI), yellow, m. 104°. V, Ac2O and NaOAc yield, after purification of the product from dilute EtOH, 4-nitro-3',6'-diacetoxybiphenyl, m. 145°. VI (2 g.) and Sn in concentrated HCl yield, after purification of the product from dilute EtOH, 4-amino-3',6'-dimethoxybiphenyl, m. 145°. HCl salt (VII), m. 225°. Picrate, m. 184°. Azo dye from resorcinol (VIII), blood-red (from dilute EtOH), m. 105°. VII (1 g.) in 0.1 N HCl and aqueous NaNO2 (0.3 g. in 10 cc.) below 5° yields, after destruction of the excess HNO2 by urea, heating 15 min. on a water bath, and purification of the product by water, 4-hydroxy-3',6'-dimethoxybiphenyl, m. 158°. IV (1 g.) in 10 cc. Ac2O and 0.1 cc. concentrated H2SO4 yield 4-nitro-3',4',6'-triacetoxybiphenyl (IX), m. 130°. Diazotization of I and condensation with III yields, after purification by EtOH, m-nitrophenylquinone (X), m. 104°. Reduction of X by SO2 and purification of the product by water yield 3-nitro-3',6'-dihydroxybiphenyl (XI), bright yellow, m. 83°. Methylation of XI and purification by 60% EtOH yield 3-nitro-3',6'-dimethoxybiphenyl (XII), lemon-yellow, m. 84°. Acetylation of X yields 3-nitro-3',6'-diacetoxybiphenyl, m. 100°. Reduction of XII by Sn and HCl yields 3-amino-3',6'-dimethoxybiphenyl, decomps. in air. HCl salt, m. 190°. Azo dye from VIII, m. 96°. Prepared like IX, 3-nitro-3',4',6'-triacetoxybiphenyl m. approx. 60°. Diazotization of 2 g. sulfanilamide by 1.5 g. KNO2 and 10 cc. dilute HCl, decomposition of the product by 6 g. NaOAc, condensation with alc. III (1.8 g. in 30 cc.), and purification of the product by dilute EtOH, yield p-sulfamylphenylquinone, brown, m. 204°.

IT 80632-65-1P, 2,4,5-Biphenyltriol, 4'-nitro-, triacetate
855253-94-0P, 2,4,5-Biphenyltriol, 3'-nitro-, triacetate
RL: PREP (Preparation)
(preparation of)

RN 80632-65-1 CAPLUS
CN [1,1'-Biphenyl]-2,4,5-triol, 4'-nitro-, triacetate (ester) (9CI) (CA INDEX NAME)



RN 855253-94-0 CAPLUS
CN [1,1'-Biphenyl]-2,4,5-triol, 3'-nitro-, 2,4,5-triacetate (CA INDEX NAME)



L19 ANSWER 52 OF 52 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1934:11102 CAPLUS Full-text
DOCUMENT NUMBER: 28:11102
ORIGINAL REFERENCE NO.: 28:1337e-i,1338a-b
TITLE: Formation of complex oxidation and condensation products of phenols-origin and nature of humic acid. II. Coupling of simple phenols and quinones to biphenyl derivatives
AUTHOR(S): Erdtman, H. G. H.
SOURCE: Proceedings of the Royal Society of London, Series A: Mathematical, Physical and Engineering Sciences (1933), 143, 191-222
CODEN: PRLAAZ; ISSN: 1364-5021
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

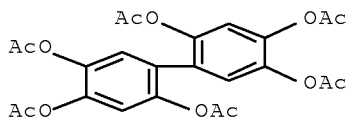
AB Pyrogallol shaken with baryta solution for 5 min. gives 2,3,4,2',3',4'-hexahydroxybiphenyl (I), m. 310-20° (decomposition); hexacetate, m. 163-4°, hexa-Me ether, m. 123°. Bipyrogallol hexa-Me ether brominated in CHCl3 gives a dibromohexamethyl ether, m. 110-1°. Pyrogallol tri-Me ether with I and HgO gives 72% of 4-iodopyrogallol tri-Me ether (II), m. 40-2°. Heated with Cu powder, II yields 2,3,4,2',3',4'-hexamethoxybiphenyl, m. 110-1°. Electrolytic oxidation of pyrogallol gave neg. results. Electrolysis of pyrogallol tri-Me ether in Me2CO and 2 N H2SO4 gives 2,6-dimethoxybiquinone, m. 255°; diacetate, m. 133°. Methoxyquinone and methoxyquinol in C6H6 gives on evaporation methoxyquinhydrone (III), m. 97°. Thermal decomposition of III yields a coupled product which on oxidation yields 4,4'-dimethoxybiquinone (IV), m. 212-14° . In Ac2O and H2SO4 IV gives 2(?),3,6,-2'(?),3',6'-hexaacetoxy-4,4'-dimethoxybiphenyl. HCl (2 mols) adds to IV, giving a chlorophenol which on boiling with Ac2O gives an anhydride (?), m. 253°. HI and PhNHNH2 reduce IV to 4,4'-dimethoxybiquinol (V), m. 210°; tetraacetate (VI), m. 186-7°. Hydrolysis and subsequent methylation of VI yields 2,4,5,2',4',5'-hexamethoxybiphenyl (VII), m. 177-9°. VI, refluxed with HBr, gives 2,3,6,7-tetraacetoxybiphenylene oxide (VIII),m. 262°. Hydrolysis of VIII yields 2,4,5,2',4',5'- hexaacetoxybiphenyl, m. 172-4°. Hydroxyquinol tri-Me ether and ICl, or H2Cr2O7 solution yields VII. Anodic oxidation of the same ether

in strongly or weakly acid solution also gives VII. Dehydrovanillin with H2O2 in acetylating solution forms 3,3'-dimethoxybiquinol (tetraacetate) (VIII), m. 176-8°. Bromination of VIII in AcOH gives 6,6'-dibromo-3,3'-dimethoxybiquinol tetraacetate, m. 207-8°. Hydrolysis of VIII results in 2,3,5,2',3',5'-hexamethoxybiphenyl (IX), m. 119-20°. Bromination of IX in CHCl3 gives the 6,6'-di-Br derivative (X), m. 271-2°. 6,6'-Dinitro derivative of IX, m. 300-1°. Nitration of X yields 6,6'-dibromo-3,3'-dimethoxybiquinone, m. 240-2° (decomposition). Toluquinol di-Me ether (XI), nitrated, gives the 5-nitro derivative, m. 117-8°. 5-I derivative m. 85°. With C5H5N, Ac2O and Zn dust, 4,4'-ditoluquinone gives tetraacetoxybitolyl, m. 137°, hydrolyzed and methylated to give 2,5,2',5'-tetramethoxy-4,4'-dimethylbiphenyl, m. 135-6°. Reduction of Nietzki's quinone with SO2 gives 2,2'-diethoxy-5,5'-dimethoxy-4,4'- dimethylbiphenyl, m. 116-8°. Methylation of Noelting's reduced quinone gives 2,2'-dimethoxy-5,5'-diethoxy-4,4'-dimethylbiphenyl, m. 94-6°. Bitoluquinone with Ac2O and H2SO4 yields 2(?),3,6,2'(?),3',6'-hexaacetoxy- 4,4'-dimethylbiphenyl, m. 202-3°. Reduction of nitroquinol dibenzyl ether gives the amino derivative (XII), m. 100-2°; Ac derivative, m. 86-7°. Fusion of XII and p-NO2C6H4CHO yields the p-nitrobenzylidene derivative; m. 105°. The following derivs. of 2-iodo-4-nitroaniline were prepared: p-nitrobenzylidene, m. 194-6°, m-nitrobenzylidine, m. 177-8°.

IT 7461-76-9P, 2,2',4,4',5,5'-Biphenylhexol, hexaacetate
RL: PREP (Preparation)
(preparation of)

RN 7461-76-9 CAPLUS

CN [1,1'-Biphenyl]-2,2',4,4',5,5'-hexol, hexaacetate (9CI) (CA INDEX NAME)



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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-41.60	-41.60

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